

10/597,241

=> d his

(FILE 'HOME' ENTERED AT 14:37:10 ON 17 AUG 2009)

FILE 'REGISTRY' ENTERED AT 14:37:22 ON 17 AUG 2009

L1 STRUCTURE UPLOADED
L2 3 S L1
L3 139 S L1 SSS FUL
L4 102 S L3 AND 6-6-6-6/SZ
L5 37 S L3 NOT L4
L6 448 S C63N?/RF
L7 37 S L5 AND L6
L8 87 S L4 AND CAPLUS/LC
L9 15 S L4 NOT L8

FILE 'CAPLUS' ENTERED AT 14:43:08 ON 17 AUG 2009

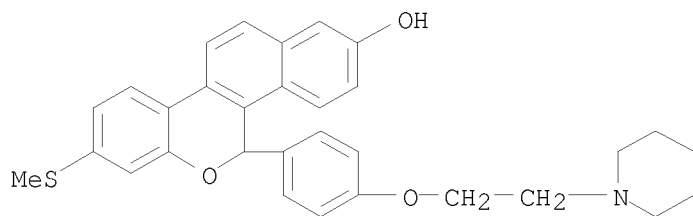
L10 21 S L4

FILE 'REGISTRY' ENTERED AT 14:43:31 ON 17 AUG 2009

=> d 19 15

10/597,241

L9 ANSWER 15 OF 15 REGISTRY COPYRIGHT 2009 ACS on STN
RN 862073-04-9 REGISTRY
ED Entered STN: 30 Aug 2005
CN 5H-Benzo[b]naphtho[2,1-d]pyran-2-ol,
8-(methylthio)-5-[4-[2-(1-piperidinyl)ethoxy]phenyl]- (CA INDEX NAME)
MF C31 H31 N O3 S
CI COM
SR CA



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

10/597,241

=> => d his

(FILE 'HOME' ENTERED AT 14:37:10 ON 17 AUG 2009)

FILE 'REGISTRY' ENTERED AT 14:37:22 ON 17 AUG 2009

L1 STRUCTURE UPLOADED
L2 3 S L1
L3 139 S L1 SSS FUL
L4 102 S L3 AND 6-6-6-6/SZ
L5 37 S L3 NOT L4
L6 448 S C63N?/RF
L7 37 S L5 AND L6
L8 87 S L4 AND CAPLUS/LC
L9 15 S L4 NOT L8

FILE 'CAPLUS' ENTERED AT 14:43:08 ON 17 AUG 2009

L10 21 S L4

FILE 'REGISTRY' ENTERED AT 14:43:31 ON 17 AUG 2009

FILE 'CAPLUS' ENTERED AT 14:44:54 ON 17 AUG 2009

L11 15 S L10 NOT (2009/SO OR 2008/SO OR 2007/SO OR 2006/SO)

=> d ibib abs hitstr total

L11 ANSWER 1 OF 15 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2008:1007107 CAPLUS

DOCUMENT NUMBER: 149:315569

TITLE: Therapeutic release agents, esters of alkylcarbamic acids, as inhibitors of fatty acid amide hydrolase activity

INVENTOR(S): Dasse, Olivier; Parrott, Jeff A.; Putman, David; Adam, Julia

PATENT ASSIGNEE(S): N.V. Organon, Neth.

SOURCE: PCT Int. Appl., 250pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2008100977	A2	20080821	WO 2008-US53785	20080213
WO 2008100977	A3	20081218		
W:	AE, AG, AL, AM, AO, AT, AU, AZ, BA, BB, BG, BH, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DO, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, GT, HN, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LA, LC, LK, LR, LS, LT, LU, LY, MA, MD, ME, MG, MK, MN, MW, MX, MY, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RS, RU, SC, SD, SE, SG, SK, SL, SM, SV, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW			
RW:	AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HR, HU, IE, IS, IT, LT, LU, LV, MC, MT, NL, NO, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AP, EA, EP, OA			

PRIORITY APPLN. INFO.: US 2007-889909P P 20070214

US 2007-948082P P 20070705

OTHER SOURCE(S): MARPAT 149:315569

AB Pharmacol. inhibition of fatty acid amide hydrolase (FAAH) activity leads to increased levels of fatty acid amides. Esters of alkylcarbamic acids are disclosed that are inhibitors of FAAH activity. Compds. disclosed herein inhibit FAAH activity. Described herein are processes for the preparation of esters of alkylcarbamic acid compds., compns. that include them, and methods of use thereof. Thus, to prepare a parenteral pharmaceutical composition for injection, 100 mg of a water-soluble salt of a compound of the invention was dissolved in DMSO and mixed with 10 mL of 0.9% sterile saline; the mixture was incorporated into dosage form unit suitable for administration by injection.

IT 188824-17-1D, LY357489, derivs.

RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(therapeutic release agents, esters of alkylcarbamic acids, as inhibitors of fatty acid amide hydrolase activity)

RN 188824-17-1 CAPLUS

CN 5H-Benzo[b]naphtho[2,1-d]pyran-2,8-diol,
5-[4-[2-(1-piperidinyl)ethoxy]phenyl]- (CA INDEX NAME)

L11 ANSWER 2 OF 15 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2005:732663 CAPLUS

DOCUMENT NUMBER: 143:193907

TITLE: Preparation of 5H-6-oxa-chrysene derivatives as selective estrogen receptor modulators

INVENTOR(S): Dodge, Jeffrey Alan; Hopkins, Randall Bruce; Wallace, Owen Brendan

PATENT ASSIGNEE(S): Eli Lilly and Company, USA

SOURCE: PCT Int. Appl., 48 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

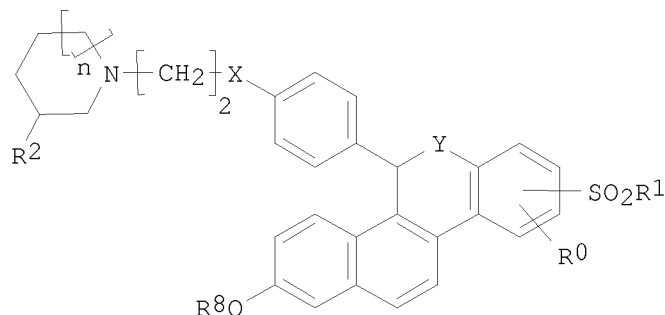
LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005073244	A1	20050811	WO 2005-US19	20050118
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
EP 1713820	A1	20061025	EP 2005-704873	20050118
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK, IS				
US 20080221163	A1	20080911	US 2006-597090	20060711
PRIORITY APPLN. INFO.:			US 2004-538302P	P 20040122
			WO 2005-US19	W 20050118
OTHER SOURCE(S):		CASREACT 143:193907; MARPAT 143:193907		

GI



AB The present invention relates to a selective estrogen receptor modulators,
 I (n = independently 0,1,2; R8 = H, SO2-alkyl, COR3; R0 = OH, CF3, C1-6

alkyl, or C1-6 alkoxy; R1 = C1-6 alkyl, C1-6 alkoxy, amine CF3, CH2CF3; R2 = H, Me; X = O or substituted amine; Y = O or S), for treating endometriosis and uterine leiomyoma.

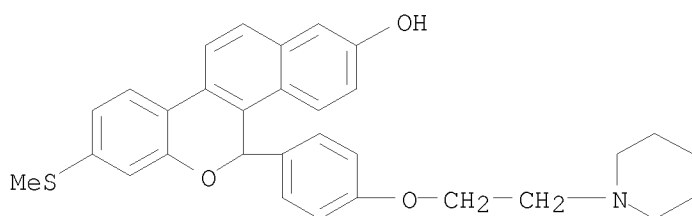
IT 861928-84-9P 861928-85-0P 861928-86-1P
861928-87-2P 861928-88-3P 861928-89-4P
861928-90-7P 861928-91-8P 861928-92-9P
861928-93-0P 861928-94-1P 861928-95-2P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of 5H-6-oxa-chrysen derivs. as selective estrogen receptor modulators)

RN 861928-84-9 CAPLUS

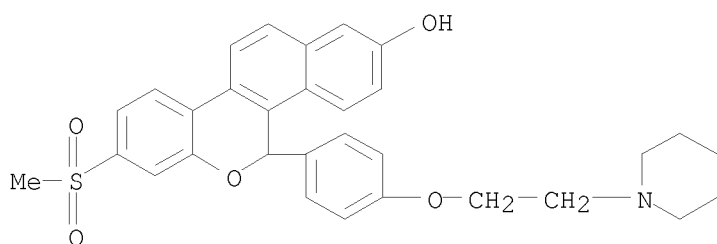
CN 5H-Benzo[b]naphtho[2,1-d]pyran-2-ol,
8-(methylthio)-5-[4-[2-(1-piperidinyl)ethoxy]phenyl]-, hydrochloride (1:1)
(CA INDEX NAME)



● HCl

RN 861928-85-0 CAPLUS

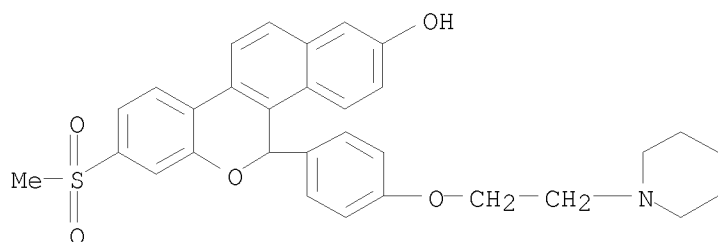
CN 5H-Benzo[b]naphtho[2,1-d]pyran-2-ol,
8-(methylsulfonyl)-5-[4-[2-(1-piperidinyl)ethoxy]phenyl]- (CA INDEX NAME)



RN 861928-86-1 CAPLUS

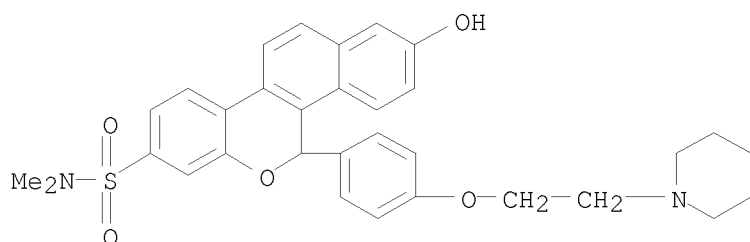
CN 5H-Benzo[b]naphtho[2,1-d]pyran-2-ol,
8-(methylsulfonyl)-5-[4-[2-(1-piperidinyl)ethoxy]phenyl]-, hydrochloride
(1:1) (CA INDEX NAME)

10/597,241



● HCl

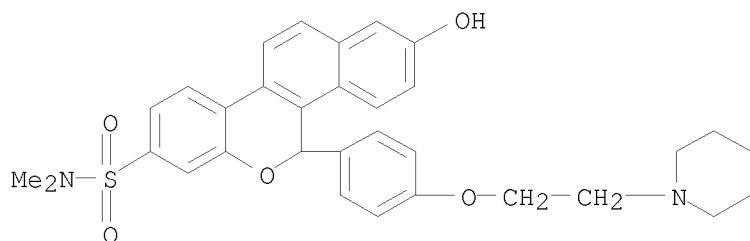
RN 861928-87-2 CAPLUS
CN 5H-Benzo[b]naphtho[2,1-d]pyran-8-sulfonamide,
2-hydroxy-N,N-dimethyl-5-[4-[2-(1-piperidinyl)ethoxy]phenyl]- (CA INDEX
NAME)



RN 861928-88-3 CAPLUS
CN 5H-Benzo[b]naphtho[2,1-d]pyran-8-sulfonamide,
2-hydroxy-N,N-dimethyl-5-[4-[2-(1-piperidinyl)ethoxy]phenyl]-,
2,2,2-trifluoroacetate (1:1) (CA INDEX NAME)

CM 1

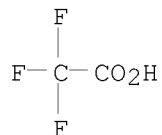
CRN 861928-87-2
CMF C32 H34 N2 O5 S



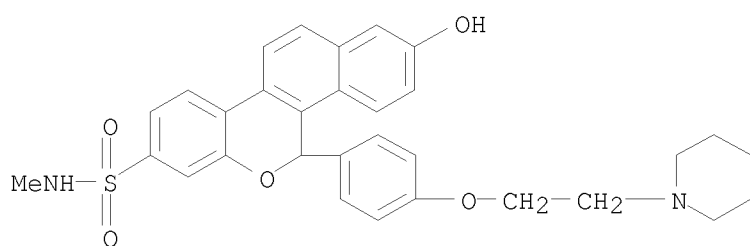
CM 2

10/597,241

CRN 76-05-1
CMF C2 H F3 O2

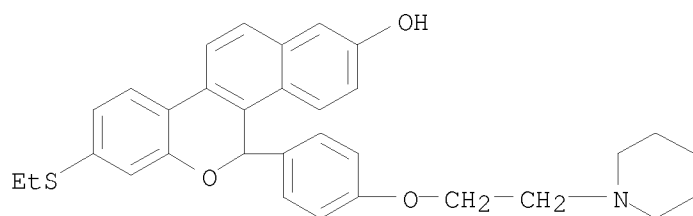


RN 861928-89-4 CAPLUS
CN 5H-Benzo[b]naphtho[2,1-d]pyran-8-sulfonamide,
2-hydroxy-N-methyl-5-[4-[2-(1-piperidinyl)ethoxy]phenyl]-, hydrochloride
(1:1) (CA INDEX NAME)



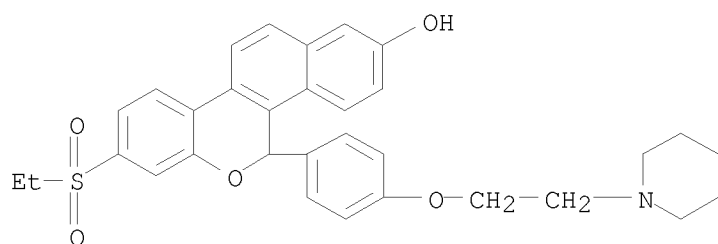
● HCl

RN 861928-90-7 CAPLUS
CN 5H-Benzo[b]naphtho[2,1-d]pyran-2-ol,
8-(ethylthio)-5-[4-[2-(1-piperidinyl)ethoxy]phenyl]- (CA INDEX NAME)

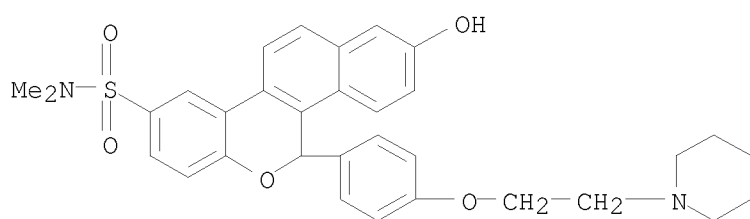


RN 861928-91-8 CAPLUS
CN 5H-Benzo[b]naphtho[2,1-d]pyran-2-ol,
8-(ethylsulfonyl)-5-[4-[2-(1-piperidinyl)ethoxy]phenyl]- (CA INDEX NAME)

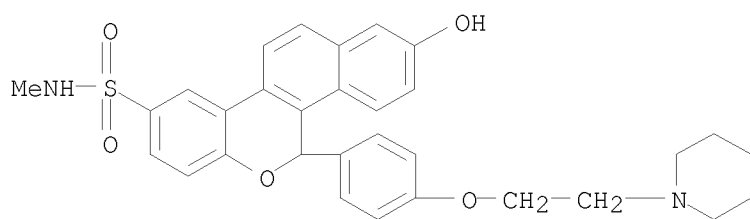
10/597,241



RN 861928-92-9 CAPLUS
CN 5H-Benzo[b]naphtho[2,1-d]pyran-9-sulfonamide,
2-hydroxy-N,N-dimethyl-5-[4-[2-(1-piperidinyl)ethoxy]phenyl]- (CA INDEX
NAME)



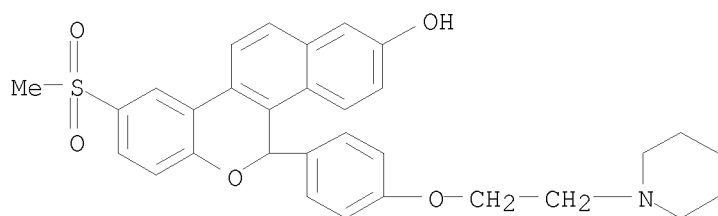
RN 861928-93-0 CAPLUS
CN 5H-Benzo[b]naphtho[2,1-d]pyran-9-sulfonamide,
2-hydroxy-N-methyl-5-[4-[2-(1-piperidinyl)ethoxy]phenyl]-, hydrochloride
(1:1) (CA INDEX NAME)



● HCl

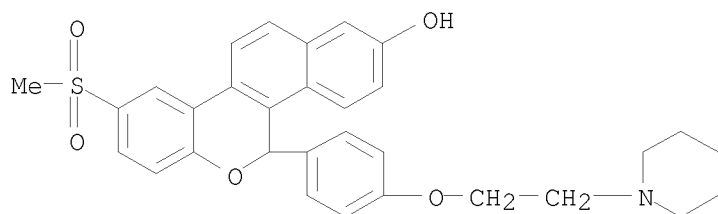
RN 861928-94-1 CAPLUS
CN 5H-Benzo[b]naphtho[2,1-d]pyran-2-ol,
9-(methylsulfonyl)-5-[4-[2-(1-piperidinyl)ethoxy]phenyl]-, hydrochloride
(1:1) (CA INDEX NAME)

10/597,241



● HCl

RN 861928-95-2 CAPLUS
CN 5H-Benzo[b]naphtho[2,1-d]pyran-2-ol,
9-(methylsulfonyl)-5-[4-[2-(1-piperidinyl)ethoxy]phenyl]- (CA INDEX NAME)



OS.CITING REF COUNT: 1 THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD
(1 CITINGS)
REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 3 OF 15 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2005:732631 CAPLUS

DOCUMENT NUMBER: 143:193912

TITLE: Preparation of piperidine derivatives as estrogen antagonists in the uterus that do not stimulate the ovaries for treating endometriosis and uterine leiomyoma

INVENTOR(S): Dally, Robert Dean; Dodge, Jeffrey Alan; Hummel, Conrad Wilson; Jones, Scott Alan; Shepherd, Timothy Alan; Wallace, Owen Brendan; Weber, Wayne Woodrow, II

PATENT ASSIGNEE(S): Eli Lilly and Company, USA

SOURCE: PCT Int. Appl., 112 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005073205	A1	20050811	WO 2005-US21	20050118
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW			
RW:	BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
EP 1709022	A1	20061011	EP 2005-704875	20050118
R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK, IS			
US 20070111988	A1	20070517	US 2006-597008	20060706
PRIORITY APPLN. INFO.:			US 2004-538441P	P 20040122
			US 2004-582945P	P 20040625
			WO 2005-US21	W 20050118
OTHER SOURCE(S):	CASREACT 143:193912; MARPAT 143:193912			
GI				

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The present invention relates to alcs. (shown as I; variables defined below; e.g. [4-[6-methoxy-1-[4-[2-(piperidin-1-yl)ethoxy]phenoxy]naphthalen-2-yl]phenyl]methanol) or a pharmaceutical acid addition salt thereof and carboxy compds. (shown as II; variables defined below; e.g. 3-[6-hydroxy-1-[4-[2-(piperidin-1-yl)ethoxy]phenoxy]naphthalen-2-yl]-N,N-dimethylbenzamide hydrochloride) or a pharmaceutical salt thereof as selective estrogen receptor modulators, useful, e.g., for treating endometriosis and/or uterine leiomyoma/leiomyomata. Other similar Markush formulas for claimed compds. are given in the claims. In the Ishikawa cell proliferation assay, cell

proliferation (using an alkaline phosphatase readout) was measured in both an agonist mode in the presence of I or II alone, and in an antagonist mode in which the ability of I or II to block estradiol stimulation of growth was measured. In the agonist mode, the compds. of 14 examples were tested and are less stimulatory than tamoxifen. For example, 3-[6-hydroxy-1-[4-[2-(piperidin-1-yl)ethoxy]phenoxy]naphthalen-2-yl]-N,N-dimethylbenzamide hydrochloride had a relative % efficacy of 15% and 2-hydroxy-5-[4-[2-(piperidin-1-yl)ethoxy]phenyl]-5H-6-oxachrysene-7-carboxylic acid trifluoroacetate had a relative % efficacy of 25%. In the antagonist mode, these same compds. inhibited greater than at least 80% of the 1 nM estradiol response. For example, 3-[6-hydroxy-1-[4-[2-(piperidin-1-yl)ethoxy]phenoxy]naphthalen-2-yl]-N,N-dimethylbenzamide hydrochloride had an IC₅₀ of 9 nM and a % efficacy of 95% and 2-hydroxy-5-[4-[2-(piperidin-1-yl)ethoxy]phenyl]-5H-6-oxachrysene-7-carboxylic acid trifluoroacetate had an IC₅₀ of 36 nM and a % efficacy of 92%. Results of a 3-day rat uterus antagonist assay are also reported. One example compound was tested in a 4-day OVX rat uterine agonist assay and did not cause any dose-related statistically significant increase in uterine eosinophil peroxidase activity. Two example compds. did not significantly elevate circulating estradiol or LH levels. For I: m = 0-2; R₀ is H, F or OH; R₁ is H, SO₂(n-C₄-C₆ alkyl) or COR₄; R₂ is H or Me provided that if m is 1 or 2, then R₂ must be H and that if m is 0, then R₂ must be Me; X is O or NR₅; Y is S or CH:CH; R₄ is C₁-C₆ alkyl, C₁-C₆ alkoxy, NR₆R₇, phenoxy, or Ph (un)substituted with halo; R₅ is H or C₁-C₆ alkyl; R₆ and R₇ = H, C₁-C₆ alkyl or phenyl; R is H and X₁ is O, CH₂ or CO or R combines with X₁ to form III (X₂ is O or S); and R₃ and R_{3a} = H or C₁-C₆ alkyl. For II: m = 0-2; R₁ is H, SO₂(n-C₄-C₆ alkyl) or COR₄; R₂ is H or Me provided that if m is 1 or 2, then R₂ must be H and that if m is 0, then R₂ must be Me; X is O or NR₅; Y is S or CH:CH; R₄ is C₁-C₆ alkyl, C₁-C₆ alkoxy, NR₆R₇, phenoxy, or Ph (un)substituted with halo; R₅ is H or C₁-C₆ alkyl; R₆ and R₇ = H, C₁-C₆ alkyl or phenyl; R is H and X₁ is O, CH₂ or CO or R combines with X₁ to form IV (X₂ is O or S); R_{3b} is NR₈R₉ or OR₁₀ or when R is H, R_{3b} may combine with the Ph with which it is attached to form V (W and W₁ are CH₂ or C:O provided that at least one of W or W₁ must be C:O; X₃ is NR₁₁ or O; R₈ and R₉ = H or C₁-C₆ alkyl or R₈ and R₉ may combine with the N to which they are both attached to form a morpholino, pyrrolidino or piperidino ring; R₁₀ and R₁₁ = H or C₁-C₆ alkyl). Although the methods of preparation are not claimed, .apprx.70 example preps. are included. For example, 3-[6-hydroxy-1-[4-[2-(piperidin-1-yl)ethoxy]phenoxy]naphthalen-2-yl]benzamide hydrochloride was prepared (88 %) by HCl treatment of 3-[6-hydroxy-1-[4-[2-(piperidin-1-yl)ethoxy]phenoxy]naphthalen-2-yl]benzonitrile hydrochloride, which was prepared (98 %) by coupling trifluoromethanesulfonic acid 6-methoxy-1-[4-[2-(piperidin-1-yl)ethoxy]phenoxy]naphthalen-2-yl ester (preparation described) with 3-cyanophenylboronic acid followed by conversion of the OMe to OH group.

IT 862081-86-5P, 8-Hydroxymethyl-5-[4-[2-(piperidin-1-yl)ethoxy]phenyl]-5H-6-oxachrysen-2-ol

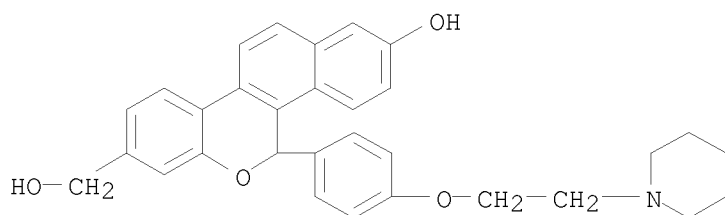
RL: PAC (Pharmacological activity); PEP (Physical, engineering or chemical process); PYP (Physical process); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); PROC (Process); USES (Uses)

(drug candidate, chromatog. resolution; preparation of piperidine derivs. as estrogen antagonists in the uterus that do not stimulate the ovaries for treating endometriosis and uterine leiomyoma)

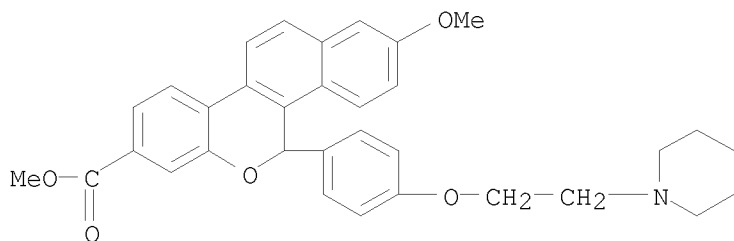
RN 862081-86-5 CAPLUS

CN 5H-Benzo[b]naphtho[2,1-d]pyran-8-methanol,

2-hydroxy-5-[4-[2-(1-piperidinyloxy)ethoxy]phenyl]- (CA INDEX NAME)

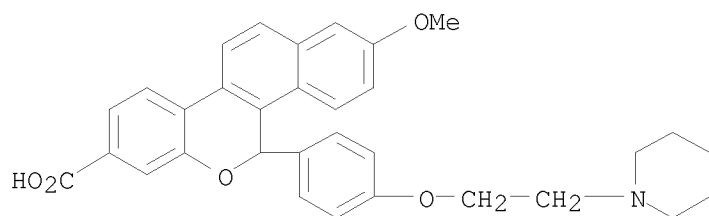


IT 862081-64-9P, 2-Methoxy-5-[4-[2-(piperidin-1-yl)ethoxy]phenyl]-5H-6-oxachrysen-8-carboxylic acid methyl ester 862081-66-1P, 2-Methoxy-5-[4-[2-(piperidin-1-yl)ethoxy]phenyl]-5H-6-oxachrysen-8-carboxylic acid ammonium salt 862081-69-4P, 2-Methoxy-5-[4-[2-(piperidin-1-yl)ethoxy]phenyl]-5H-6-oxachrysen-8-carboxamide 862081-77-4P, 2-Methoxy-5-[4-[2-(piperidin-1-yl)ethoxy]phenyl]-5H-6-oxachrysen-8-carboxylic acid methylamine salt 862081-85-4P, [2-Methoxy-5-[4-[2-(piperidin-1-yl)ethoxy]phenyl]-5H-6-oxachrysen-8-yl]methanol
 RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
 (drug candidate; preparation of piperidine derivs. as estrogen antagonists in the uterus that do not stimulate the ovaries for treating endometriosis and uterine leiomyoma)
 RN 862081-64-9 CAPLUS
 CN 5H-Benzo[b]naphtho[2,1-d]pyran-8-carboxylic acid, 2-methoxy-5-[4-[2-(1-piperidinyloxy)ethoxy]phenyl]-, methyl ester (CA INDEX NAME)

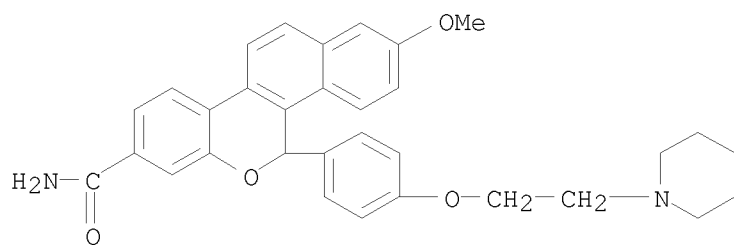


RN 862081-66-1 CAPLUS
 CN 5H-Benzo[b]naphtho[2,1-d]pyran-8-carboxylic acid, 2-methoxy-5-[4-[2-(1-piperidinyloxy)ethoxy]phenyl]-, ammonium salt (1:1) (CA INDEX NAME)

10/597,241



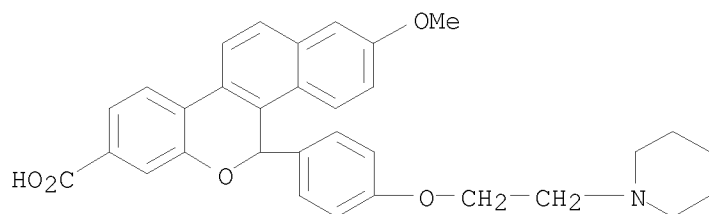
RN 862081-69-4 CAPLUS
CN 5H-Benzo[b]naphtho[2,1-d]pyran-8-carboxamide,
2-methoxy-5-[4-[2-(1-piperidinyl)ethoxy]phenyl]- (CA INDEX NAME)



RN 862081-77-4 CAPLUS
CN 5H-Benzo[b]naphtho[2,1-d]pyran-8-carboxylic acid,
2-methoxy-5-[4-[2-(1-piperidinyl)ethoxy]phenyl]-, compd. with methanamine
(1:1) (CA INDEX NAME)

CM 1

CRN 862081-76-3
CMF C32 H31 N O5

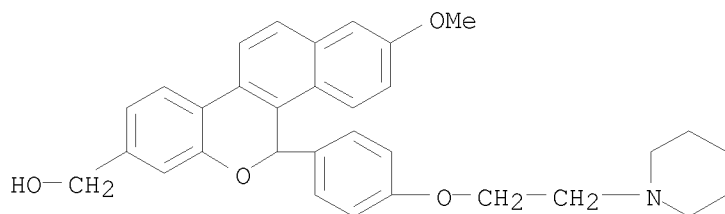


CM 2

CRN 74-89-5
CMF C H5 N

H₃C—NH₂

RN 862081-85-4 CAPLUS

CN 5H-Benzo[b]naphtho[2,1-d]pyran-8-methanol,
2-methoxy-5-[4-[2-(1-piperidinyl)ethoxy]phenyl]- (CA INDEX NAME)

IT 862081-65-0P, 2-Hydroxy-5-[4-[2-(piperidin-1-yl)ethoxy]phenyl]-
5H-6-oxachrysene-8-carboxylic acid ammonium salt 862081-67-2P,
2-Hydroxy-5-[4-[2-(piperidin-1-yl)ethoxy]phenyl]-5H-6-oxachrysene-8-
carboxylic acid dimethylamide 862081-70-7P,
2-Hydroxy-5-[4-[2-(piperidin-1-yl)ethoxy]phenyl]-5H-6-oxachrysene-8-
carboxamide 862081-74-1P 862081-75-2P,
2-Hydroxy-5-[4-[2-(piperidin-1-yl)ethoxy]phenyl]-5H-6-oxachrysene-9-
carboxylic acid trifluoroacetate 862081-78-5P,
2-Methoxy-5-[4-[2-(piperidin-1-yl)ethoxy]phenyl]-5H-6-oxachrysene-8-
carboxylic acid methylamide hydrochloride 862081-81-0P,
2-Hydroxy-5-[4-[2-(piperidin-1-yl)ethoxy]phenyl]-5H-6-oxachrysene-8-
carboxylic acid methylamide 862081-83-2P
862081-84-3P, 2-Hydroxy-5-[4-[2-(piperidin-1-yl)ethoxy]phenyl]-5H-
6-oxachrysene-7-carboxylic acid trifluoroacetate 862082-67-5P
862082-68-6P 862082-70-0P 862082-71-1P
862082-72-2P 862082-73-3P 862082-74-4P

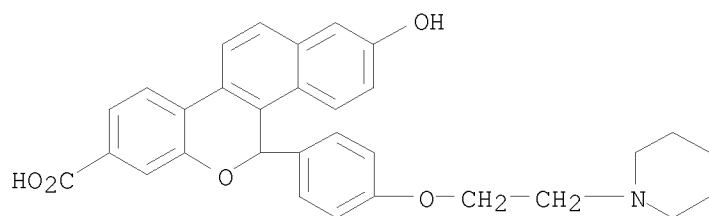
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
(Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
(Uses)

(drug candidate; preparation of piperidine derivs. as estrogen antagonists
in the uterus that do not stimulate the ovaries for treating
endometriosis and uterine leiomyoma)

RN 862081-65-0 CAPLUS

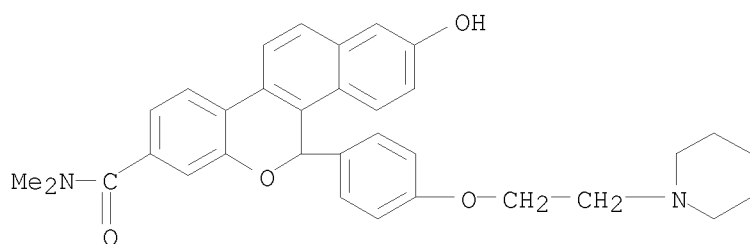
CN 5H-Benzo[b]naphtho[2,1-d]pyran-8-carboxylic acid,
2-hydroxy-5-[4-[2-(1-piperidinyl)ethoxy]phenyl]-, ammonium salt (1:1) (CA
INDEX NAME)

10/597,241

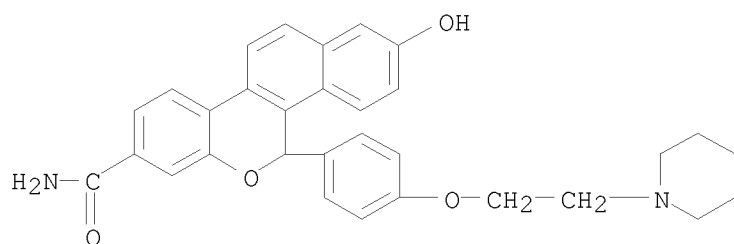


● NH₃

RN 862081-67-2 CAPLUS
CN 5H-Benzo[b]naphtho[2,1-d]pyran-8-carboxamide,
2-hydroxy-5-[4-[2-(1-piperidinyl)ethoxy]phenyl]- (CA INDEX
NAME)

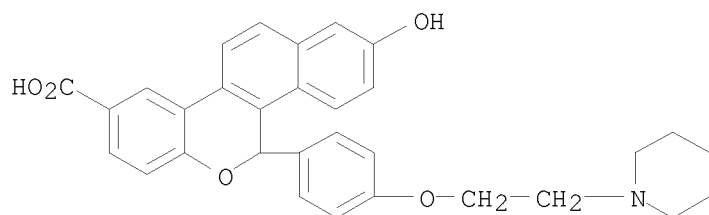


RN 862081-70-7 CAPLUS
CN 5H-Benzo[b]naphtho[2,1-d]pyran-8-carboxamide,
2-hydroxy-5-[4-[2-(1-piperidinyl)ethoxy]phenyl]- (CA INDEX NAME)



RN 862081-74-1 CAPLUS
CN 5H-Benzo[b]naphtho[2,1-d]pyran-9-carboxylic acid,
2-hydroxy-5-[4-[2-(1-piperidinyl)ethoxy]phenyl]- (CA INDEX NAME)

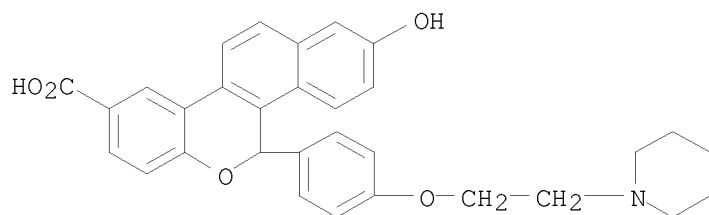
10/597,241



RN 862081-75-2 CAPLUS
CN 5H-Benzo[b]naphtho[2,1-d]pyran-9-carboxylic acid,
2-hydroxy-5-[4-[2-(1-piperidinyl)ethoxy]phenyl]-, 2,2,2-trifluoroacetate
(1:1) (CA INDEX NAME)

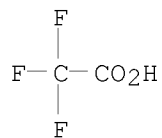
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CRN 862081-74-1
CMF C31 H29 N O5



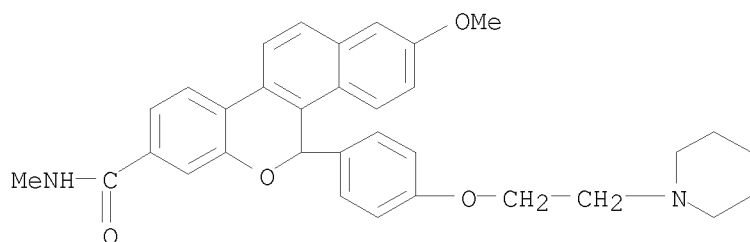
CM 2

CRN 76-05-1
CMF C2 H F3 O2



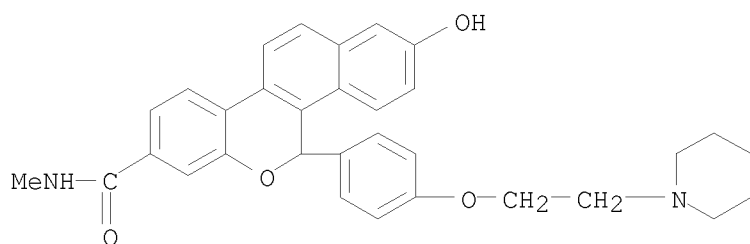
RN 862081-78-5 CAPLUS
CN 5H-Benzo[b]naphtho[2,1-d]pyran-8-carboxamide,
2-methoxy-N-methyl-5-[4-[2-(1-piperidinyl)ethoxy]phenyl]-, hydrochloride
(1:1) (CA INDEX NAME)

10/597,241

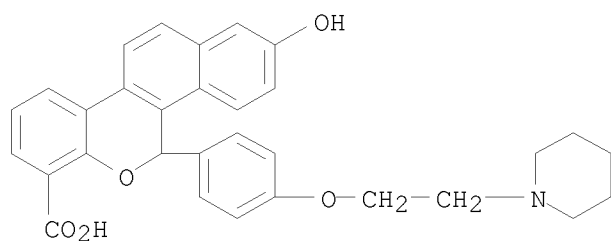


● HCl

RN 862081-81-0 CAPLUS
CN 5H-Benzo[b]naphtho[2,1-d]pyran-8-carboxamide,
2-hydroxy-N-methyl-5-[4-[2-(1-piperidinyl)ethoxy]phenyl]- (CA INDEX NAME)



RN 862081-83-2 CAPLUS
CN 5H-Benzo[b]naphtho[2,1-d]pyran-7-carboxylic acid,
2-hydroxy-5-[4-[2-(1-piperidinyl)ethoxy]phenyl]- (CA INDEX NAME)

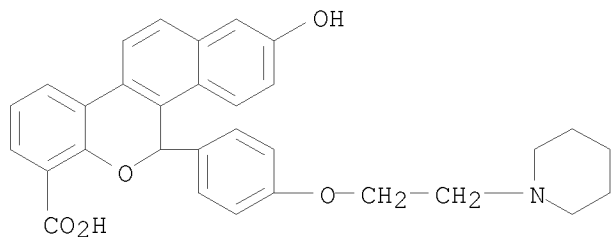


RN 862081-84-3 CAPLUS
CN 5H-Benzo[b]naphtho[2,1-d]pyran-7-carboxylic acid,
2-hydroxy-5-[4-[2-(1-piperidinyl)ethoxy]phenyl]-, 2,2,2-trifluoroacetate
(1:1) (CA INDEX NAME)

CM 1

CRN 862081-83-2
CMF C31 H29 N O5

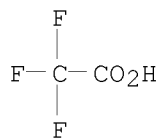
10/597,241



CM 2

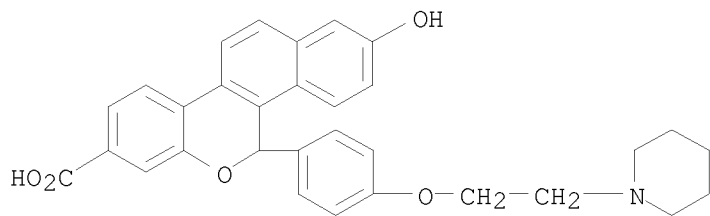
CRN 76-05-1

CMF C2 H F3 O2



RN 862082-67-5 CAPLUS

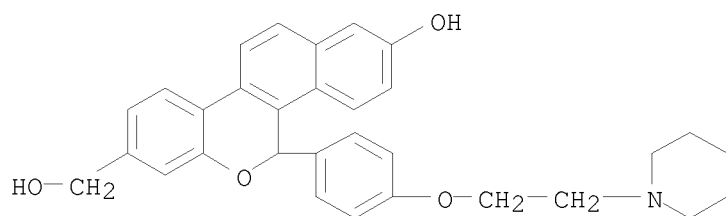
CN	5H-Benzo[b]naphtho[2,1-d]pyran-8-carboxylic acid, 2-hydroxy-5-[4-[2-(1-piperidinyl)ethoxy]phenyl]-	(CA INDEX NAME)
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RN 862082-68-6 CAPLUS

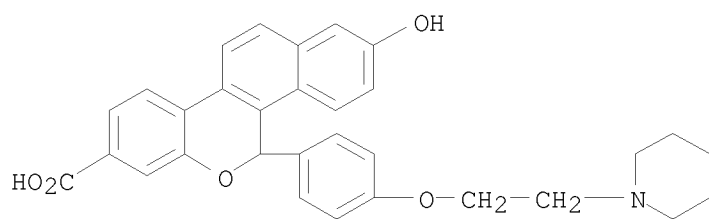
CN 5H-Benzo[b]naphtho[2,1-d]pyran-8-methanol,
2-hydroxy-5-[4-[2-(1-piperidinyl)ethoxy]phenyl]-, hydrochloride (1:1) (CA
INDEX NAME)

10/597,241



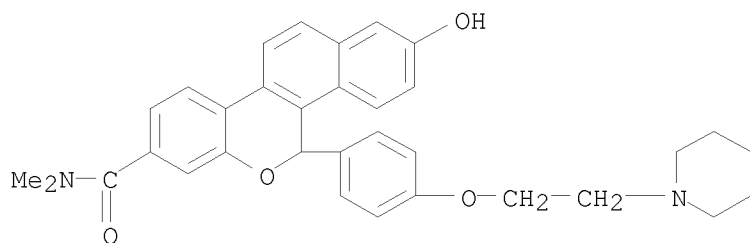
● HCl

RN 862082-70-0 CAPLUS
CN 5H-Benzo[b]naphtho[2,1-d]pyran-8-carboxylic acid,
2-hydroxy-5-[4-[2-(1-piperidinyl)ethoxy]phenyl]-, hydrochloride (1:1) (CA
INDEX NAME)



● HCl

RN 862082-71-1 CAPLUS
CN 5H-Benzo[b]naphtho[2,1-d]pyran-8-carboxamide,
2-hydroxy-N,N-dimethyl-5-[4-[2-(1-piperidinyl)ethoxy]phenyl]-,
hydrochloride (1:1) (CA INDEX NAME)

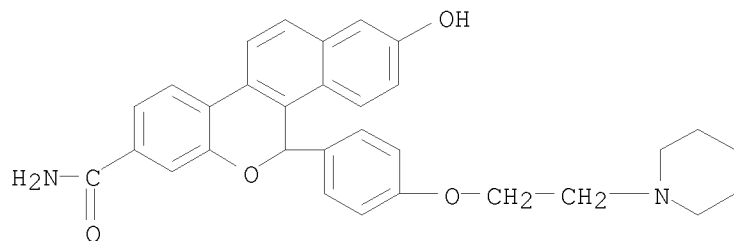


● HCl

RN 862082-72-2 CAPLUS

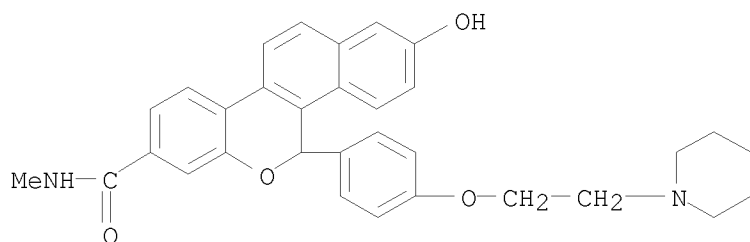
10/597,241

CN 5H-Benzo[b]naphtho[2,1-d]pyran-8-carboxamide,
2-hydroxy-5-[4-[2-(1-piperidinyloxy)]phenyl]-, hydrochloride (1:1) (CA
INDEX NAME)



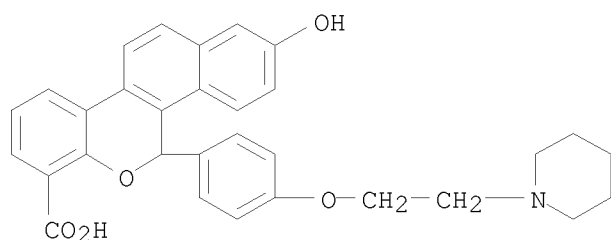
● HCl

RN 862082-73-3 CAPLUS
CN 5H-Benzo[b]naphtho[2,1-d]pyran-8-carboxamide,
2-hydroxy-N-methyl-5-[4-[2-(1-piperidinyloxy)]phenyl]-, hydrochloride
(1:1) (CA INDEX NAME)



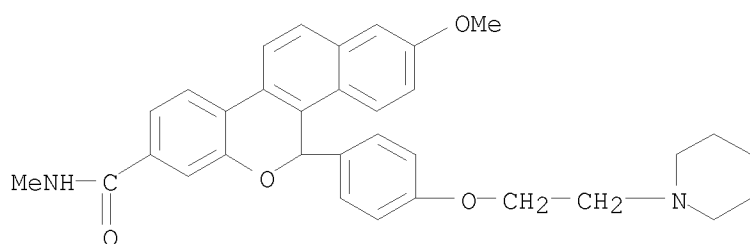
● HCl

RN 862082-74-4 CAPLUS
CN 5H-Benzo[b]naphtho[2,1-d]pyran-7-carboxylic acid,
2-hydroxy-5-[4-[2-(1-piperidinyloxy)]phenyl]-, hydrochloride (1:1) (CA
INDEX NAME)



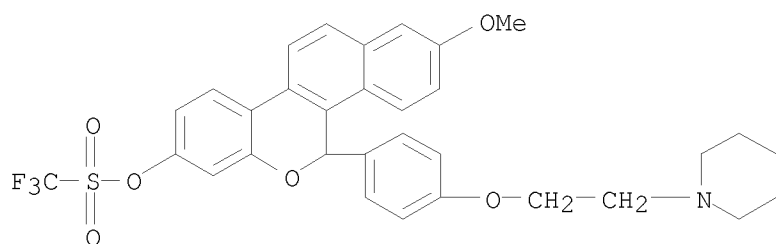
● HCl

IT 862081-80-9, 2-Methoxy-5-[4-[2-(piperidin-1-yl)ethoxy]phenyl]-5H-6-oxachrysen-8-carboxylic acid methylamide
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (preparation of piperidine derivs. as estrogen antagonists in the uterus that do not stimulate the ovaries for treating endometriosis and uterine leiomyoma)
 RN 862081-80-9 CAPLUS
 CN 5H-Benzo[b]naphtho[2,1-d]pyran-8-carboxamide, 2-methoxy-N-methyl-5-[4-[2-(1-piperidinyl)ethoxy]phenyl]- (CA INDEX NAME)

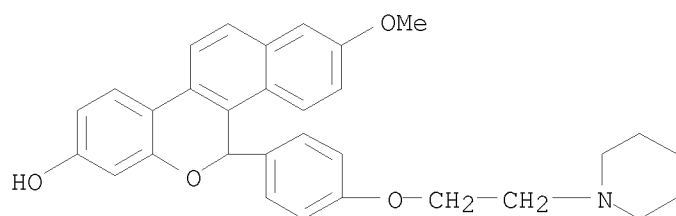


IT 862081-60-5P, Trifluoromethanesulfonic acid 2-methoxy-5-[4-[2-(piperidin-1-yl)ethoxy]phenyl]-5H-6-oxachrysen-8-yl ester 862081-61-6P, 2-Methoxy-5-[4-[2-(piperidin-1-yl)ethoxy]phenyl]-5H-6-oxachrysen-8-ol 862081-68-3P, 2-Methoxy-5-[4-[2-(piperidin-1-yl)ethoxy]phenyl]-5H-6-oxachrysen-8-carbonitrile 1023717-25-0P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (preparation of piperidine derivs. as estrogen antagonists in the uterus that do not stimulate the ovaries for treating endometriosis and uterine leiomyoma)
 RN 862081-60-5 CAPLUS
 CN Methanesulfonic acid, 1,1,1-trifluoro-, 2-methoxy-5-[4-[2-(1-piperidinyl)ethoxy]phenyl]-5H-benzo[b]naphtho[2,1-d]pyran-8-yl ester (CA INDEX NAME)

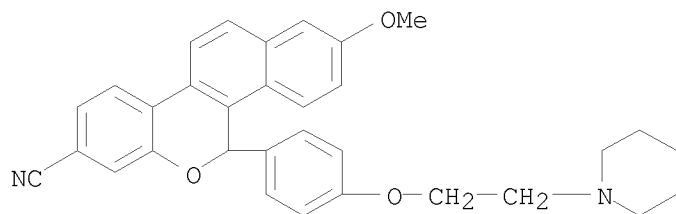
10/597,241



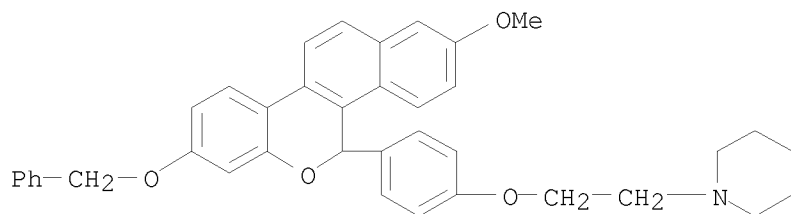
RN 862081-61-6 CAPLUS
CN 5H-Benzo[b]naphtho[2,1-d]pyran-8-ol,
2-methoxy-5-[4-[2-(1-piperidinyl)ethoxy]phenyl]- (CA INDEX NAME)



RN 862081-68-3 CAPLUS
CN 5H-Benzo[b]naphtho[2,1-d]pyran-8-carbonitrile,
2-methoxy-5-[4-[2-(1-piperidinyl)ethoxy]phenyl]- (CA INDEX NAME)



RN 1023717-25-0 CAPLUS
CN Piperidine, 1-[2-[4-[2-methoxy-8-(phenylmethoxy)-5H-benzo[b]naphtho[2,1-d]pyran-5-yl]phenoxy]ethyl]- (CA INDEX NAME)



10/597,241

OS.CITING REF COUNT:	2	THERE ARE 2 CAPLUS RECORDS THAT CITE THIS RECORD (2 CITINGS)
REFERENCE COUNT:	7	THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 4 OF 15 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2005:732630 CAPLUS

DOCUMENT NUMBER: 143:211842

TITLE: Preparation of piperidine derivatives as selective estrogen receptor modulators for the treatment of vasomotor symptoms

INVENTOR(S): Dally, Robert Dean; Dodge, Jeffrey Alan; Frank, Scott Alan; Hinklin, Ronald Jay; Shepherd, Timothy Alan; Wallace, Owen Brendan

PATENT ASSIGNEE(S): Eli Lilly and Company, USA

SOURCE: PCT Int. Appl., 139 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005073204	A1	20050811	WO 2005-US20	20050118
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2005207821	A1	20050811	AU 2005-207821	20050118
CA 2551956	A1	20050811	CA 2005-2551956	20050118
EP 1709021	A1	20061011	EP 2005-704874	20050118
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, PL, SK, BA, HR, IS, YU				
CN 1910167	A	20070207	CN 2005-80002914	20050118
BR 2005006721	A	20070502	BR 2005-6721	20050118
JP 2007519721	T	20070719	JP 2006-551097	20050118
SG 149867	A1	20090227	SG 2009-414	20050118
ZA 2006005665	A	20080528	ZA 2006-5665	20060710
US 20090023917	A1	20090122	US 2006-597241	20060718
KR 2006129277	A	20061215	KR 2006-714630	20060720
KR 849559	B1	20080731		
MX 2006008291	A	20061002	MX 2006-8291	20060721
NO 2006003760	A	20061016	NO 2006-3760	20060822
IN 2006KN02478	A	20070615	IN 2006-KN2478	20060822
KR 2008016755	A	20080221	KR 2008-703065	20080205
PRIORITY APPLN. INFO.:			US 2004-538342P	P 20040122
			US 2004-538442P	P 20040122
			WO 2005-US20	W 20050118
			KR 2006-714630	A3 20060720

OTHER SOURCE(S): CASREACT 143:211842; MARPAT 143:211842

GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

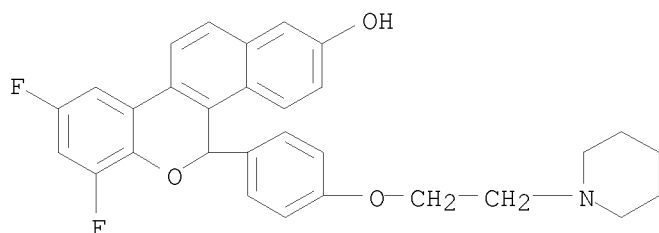
AB The present invention relates to selective estrogen receptor modulators (no data; shown as I; variables defined below; e.g. 1-[2-[4-[[2-(2,6-difluorophenyl)-6-methoxynaphthalen-1-yl]oxy]phenoxy]ethyl]piperidine (shown as II)) or pharmaceutical acid addition salts thereof useful for treating vasomotor symptoms, in particular hot flashes, night sweats and other symptoms that affect women around menopause. In a morphine withdrawal, rat hot flash model, representative I were tested ≤ 30 mg/kg PO and caused an attenuation of tail skin temperature increase, as measured by temperature change 15 min post naloxone injection

or AUC over 45 min post naloxone administration. For I: $m = 0-2$; $n = 1-4$; R is H or Me provided that if m is 1 or 2, then R must be H and that if m is 0, then R must be Me; R1 is H, SO₂(n-C₄-C₆ alkyl) or COR₂; X is O or NR₃; X1 is O, CH₂ or C=O; R₆ is H or F or R₆ combines with X1 to form III (Y is O, S, SO or NR₄; e.g. 7,9-difluoro-5-[4-[2-(piperidin-1-yl)ethoxy]phenyl]-5H-6-oxachrysen-2-ol (shown as IV)); R₂ is C₁-C₆ alkyl, C₁-C₆ alkoxy, NR₅R_{5a}, phenoxy, or Ph (un)substituted with halo; R₃ and R₄ = H or C₁-C₆ alkyl; and R₅ and R_{5a} = H, C₁-C₆ alkyl or Ph. Although the methods of preparation are not claimed, .apprx.150 example preps. are included. For example, II was prepared (32 %) from trifluoromethanesulfonic acid 6-methoxy-1-[4-[2-(piperidin-1-yl)ethoxy]phenoxy]naphthalen-2-yl ester (preparation given) and (2,6-difluorophenyl)boronic acid in DMF using potassium phosphate and tetrakis(triphenylphosphine)palladium(0).

IT 861931-21-7P, 7,9-Difluoro-5-[4-[2-(piperidin-1-yl)ethoxy]phenyl]-5H-6-oxachrysen-2-ol
 RL: PAC (Pharmacological activity); PEP (Physical, engineering or chemical process); PYP (Physical process); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); PROC (Process); RACT (Reactant or reagent); USES (Uses) (drug candidate, chromatog. resolution; preparation of piperidine derivs. as selective estrogen receptor modulators for treatment of vasomotor symptoms)

RN 861931-21-7 CAPLUS

CN 5H-Benzo[b]naphtho[2,1-d]pyran-2-ol,
 7,9-difluoro-5-[4-[2-(1-piperidinyl)ethoxy]phenyl]- (CA INDEX NAME)



IT 861931-50-2P, 7,8-Difluoro-5-[4-[2-(piperidin-1-yl)ethoxy]phenyl]-5H-6-oxachrysen-2-ol hydrochloride
 861931-55-7P, 5-[4-[2-(Azepan-1-yl)ethoxy]phenyl]-9-fluoro-5H-6-oxachrysen-2-ol 861931-58-0P,
 5-[4-[2-(Azepan-1-yl)ethoxy]phenyl]-10-fluoro-5H-6-oxachrysen-2-ol
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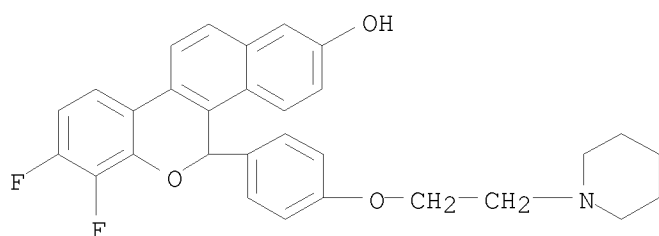
yl)ethyl]amino]phenyl]-5H-6-oxachrysen-2-ol dihydrochloride
 861931-85-3P, 8,9-Difluoro-5-[4-[2-(piperidin-1-yl)ethoxy]phenyl]-
 5H-6-oxachrysen-2-ol

RL: PAC (Pharmacological activity); PEP (Physical, engineering or chemical
 process); PYP (Physical process); SPN (Synthetic preparation); THU
 (Therapeutic use); BIOL (Biological study); PREP (Preparation); PROC
 (Process); USES (Uses)

(drug candidate, chromatog. resolution; preparation of piperidine derivs. as
 selective estrogen receptor modulators for treatment of vasomotor
 symptoms)

RN 861931-50-2 CAPLUS

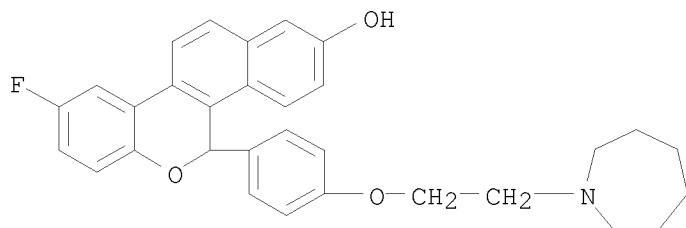
CN 5H-Benzo[b]naphtho[2,1-d]pyran-2-ol,
 7,8-difluoro-5-[4-[2-(1-piperidinyl)ethoxy]phenyl]-, hydrochloride (1:1)
 (CA INDEX NAME)



● HCl

RN 861931-55-7 CAPLUS

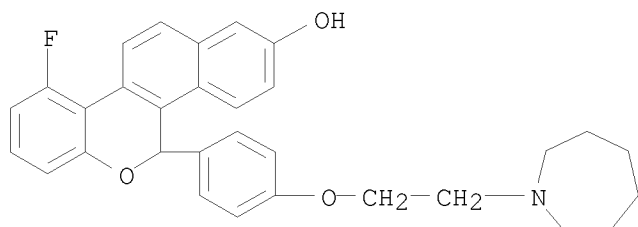
CN 5H-Benzo[b]naphtho[2,1-d]pyran-2-ol,
 9-fluoro-5-[4-[2-(hexahydro-1H-azepin-1-yl)ethoxy]phenyl]- (CA INDEX
 NAME)



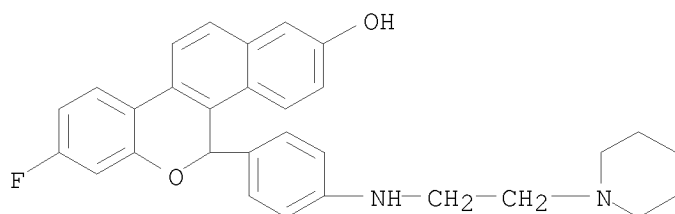
RN 861931-58-0 CAPLUS

CN 5H-Benzo[b]naphtho[2,1-d]pyran-2-ol,
 10-fluoro-5-[4-[2-(hexahydro-1H-azepin-1-yl)ethoxy]phenyl]- (CA INDEX
 NAME)

10/597,241

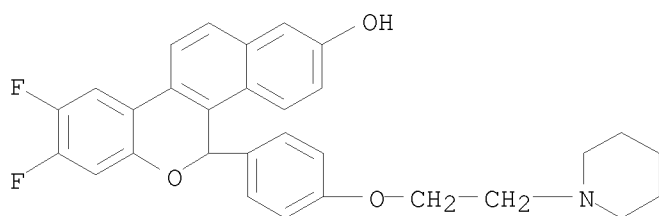


RN 861931-68-2 CAPLUS
CN 5H-Benzo[b]naphtho[2,1-d]pyran-2-ol,
8-fluoro-5-[4-[[2-(1-piperidinyloxy)ethyl]amino]phenyl]-, hydrochloride (1:2)
(CA INDEX NAME)



● 2 HCl

RN 861931-85-3 CAPLUS
CN 5H-Benzo[b]naphtho[2,1-d]pyran-2-ol,
8,9-difluoro-5-[4-[2-(1-piperidinyloxy)ethyl]amino]phenyl]- (CA INDEX NAME)

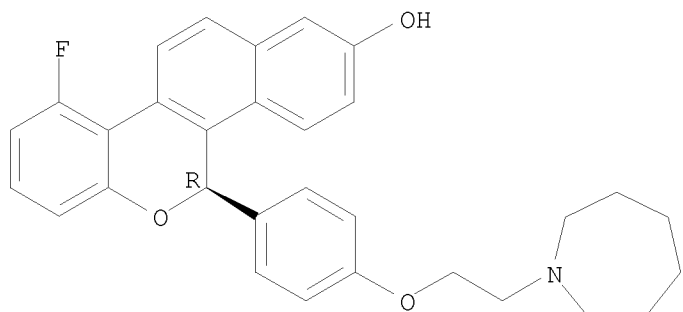


IT 861931-59-1P, (R)-5-[4-[2-(Azepan-1-yl)ethoxy]phenyl]-10-fluoro-
5H-6-oxachrysen-2-ol 861931-60-4P,
(S)-5-[4-[2-(Azepan-1-yl)ethoxy]phenyl]-10-fluoro-5H-6-oxachrysen-2-ol
RL: PAC (Pharmacological activity); PUR (Purification or recovery); SPN
(Synthetic preparation); THU (Therapeutic use); BIOL (Biological study);
PREP (Preparation); USES (Uses)
(drug candidate, chromatog. resolution; preparation of piperidine derivs. as
selective estrogen receptor modulators for treatment of vasomotor
symptoms)
RN 861931-59-1 CAPLUS
CN 5H-Benzo[b]naphtho[2,1-d]pyran-2-ol,

10/597,241

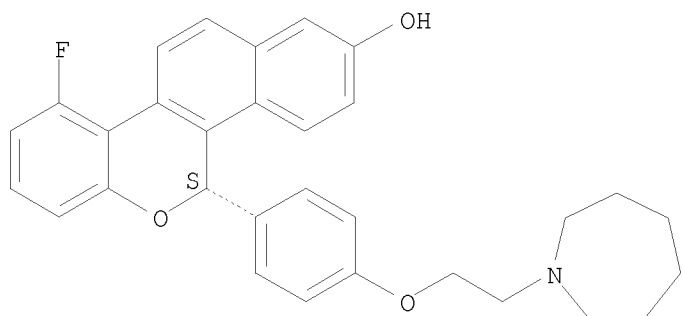
10-fluoro-5-[4-[2-(hexahydro-1H-azepin-1-yl)ethoxy]phenyl]-, (5R)- (CA INDEX NAME)

Absolute stereochemistry.



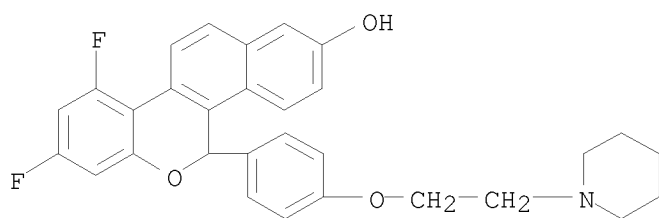
RN 861931-60-4 CAPLUS
CN 5H-Benzo[b]naphtho[2,1-d]pyran-2-ol,
10-fluoro-5-[4-[2-(hexahydro-1H-azepin-1-yl)ethoxy]phenyl]-, (5S)- (CA INDEX NAME)

Absolute stereochemistry.



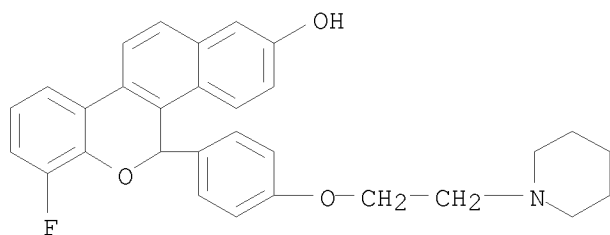
IT 861931-26-2P, 8,10-Difluoro-5-[4-[2-(piperidin-1-yl)ethoxy]phenyl]-5H-6-oxachrysen-2-ol hydrochloride
861931-46-6P, 7-Fluoro-5-[4-[2-(piperidin-1-yl)ethoxy]phenyl]-5H-6-oxachrysen-2-ol hydrochloride 861931-47-7P,
9-Fluoro-5-[4-[2-(piperidin-1-yl)ethoxy]phenyl]-5H-6-oxachrysen-2-ol hydrochloride
RL: PAC (Pharmacological activity); PEP (Physical, engineering or chemical process); PYP (Physical process); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); PROC (Process); USES (Uses)
(drug candidate, partial chromatog. resolution; preparation of piperidine derivs. as selective estrogen receptor modulators for treatment of vasomotor symptoms)
RN 861931-26-2 CAPLUS
CN 5H-Benzo[b]naphtho[2,1-d]pyran-2-ol,
8,10-difluoro-5-[4-[2-(1-piperidinyl)ethoxy]phenyl]-, hydrochloride (1:1)
(CA INDEX NAME)

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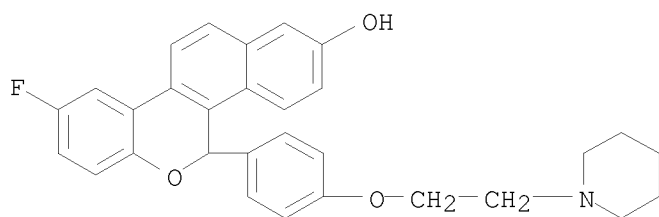
● HCl

RN 861931-46-6 CAPLUS
CN 5H-Benzo[b]naphtho[2,1-d]pyran-2-ol,
7-fluoro-5-[4-[2-(1-piperidinyl)ethoxy]phenyl]-, hydrochloride (1:1) (CA
INDEX NAME)



● HCl

RN 861931-47-7 CAPLUS
CN 5H-Benzo[b]naphtho[2,1-d]pyran-2-ol,
9-fluoro-5-[4-[2-(1-piperidinyl)ethoxy]phenyl]-, hydrochloride (1:1) (CA
INDEX NAME)



● HCl

IT 861931-48-8P, (R)-7,9-Difluoro-5-[4-[2-(piperidin-1-yl)ethoxy]phenyl]-5H-6-oxachrysen-2-ol 861931-49-9P,
(S)-7,9-Difluoro-5-[4-[2-(piperidin-1-yl)ethoxy]phenyl]-5H-6-oxachrysen-2-

ol

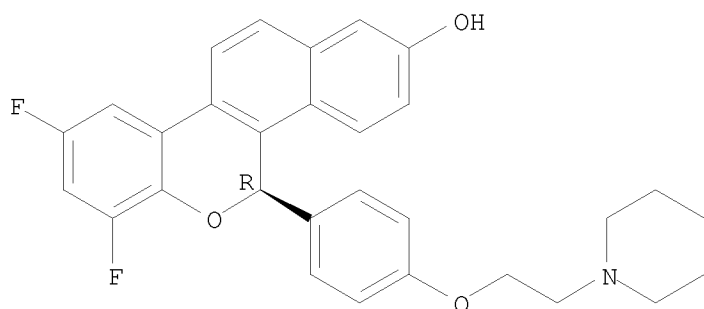
RL: PAC (Pharmacological activity); PUR (Purification or recovery); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(drug candidate, partial chromatog. resolution; preparation of piperidine derivs. as selective estrogen receptor modulators for treatment of vasomotor symptoms)

RN 861931-48-8 CAPLUS

CN 5H-Benzo[b]naphtho[2,1-d]pyran-2-ol,
7,9-difluoro-5-[4-[2-(1-piperidinyl)ethoxy]phenyl]-, (5R)- (CA INDEX NAME)

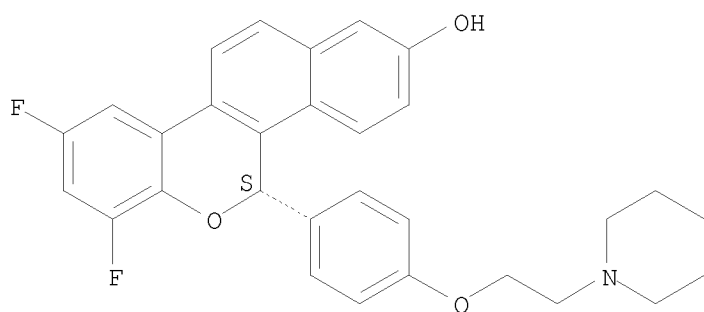
Absolute stereochemistry.



RN 861931-49-9 CAPLUS

CN 5H-Benzo[b]naphtho[2,1-d]pyran-2-ol,
7,9-difluoro-5-[4-[2-(1-piperidinyl)ethoxy]phenyl]-, (5S)- (CA INDEX NAME)

Absolute stereochemistry.



IT 861931-51-3P, (R)-7,8-Difluoro-5-[4-[2-(piperidin-1-yl)ethoxy]phenyl]-5H-6-oxachrysen-2-ol hydrochloride
861931-52-4P, (S)-7,8-Difluoro-5-[4-[2-(piperidin-1-yl)ethoxy]phenyl]-5H-6-oxachrysen-2-ol hydrochloride
861931-56-8P, (R)-5-[4-[2-(Azepan-1-yl)ethoxy]phenyl]-9-fluoro-5H-6-oxachrysen-2-ol 861931-57-9P,
(S)-5-[4-[2-(Azepan-1-yl)ethoxy]phenyl]-9-fluoro-5H-6-oxachrysen-2-ol
861931-69-3P, (R)-8-Fluoro-5-[4-[2-(piperidin-1-yl)ethyl]amino]phenyl]-5H-6-oxachrysen-2-ol dihydrochloride
861931-70-6P, (S)-8-Fluoro-5-[4-[2-(piperidin-1-

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yl)ethyl]amino]phenyl]-5H-6-oxachrysen-2-ol dihydrochloride

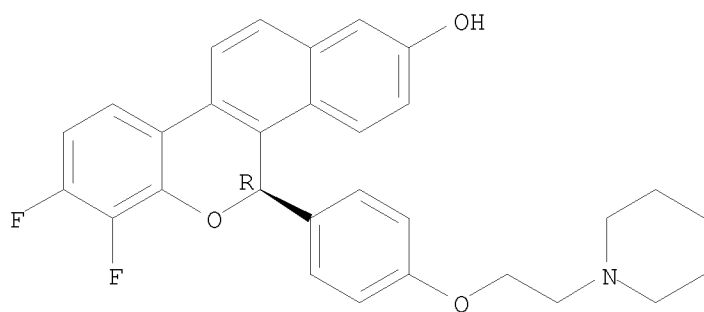
RL: PAC (Pharmacological activity); PUR (Purification or recovery); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(drug candidate; preparation of piperidine derivs. as selective estrogen receptor modulators for treatment of vasomotor symptoms)

RN 861931-51-3 CAPLUS

CN 5H-Benzo[b]naphtho[2,1-d]pyran-2-ol,
7,8-difluoro-5-[4-[2-(1-piperidinyl)ethoxy]phenyl]-, hydrochloride (1:1),
(5R)- (CA INDEX NAME)

Absolute stereochemistry.

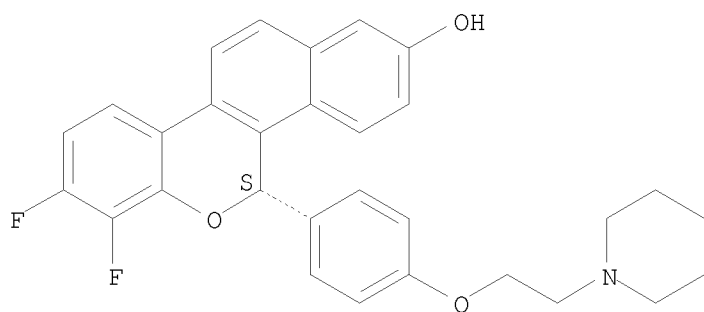


● HCl

RN 861931-52-4 CAPLUS

CN 5H-Benzo[b]naphtho[2,1-d]pyran-2-ol,
7,8-difluoro-5-[4-[2-(1-piperidinyl)ethoxy]phenyl]-, hydrochloride (1:1),
(5S)- (CA INDEX NAME)

Absolute stereochemistry.



● HCl

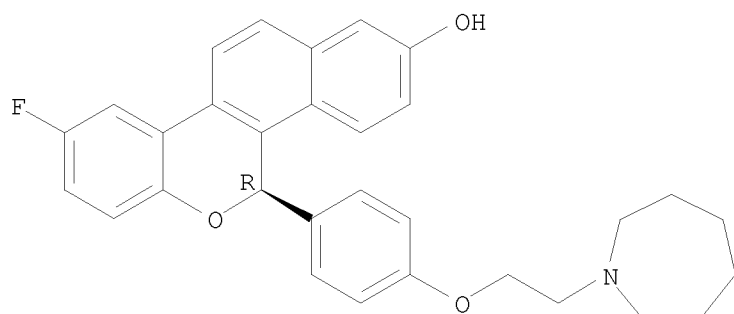
RN 861931-56-8 CAPLUS

CN 5H-Benzo[b]naphtho[2,1-d]pyran-2-ol,
9-fluoro-5-[4-[2-(hexahydro-1H-azepin-1-yl)ethoxy]phenyl]-, (5R)- (CA

10/597,241

INDEX NAME)

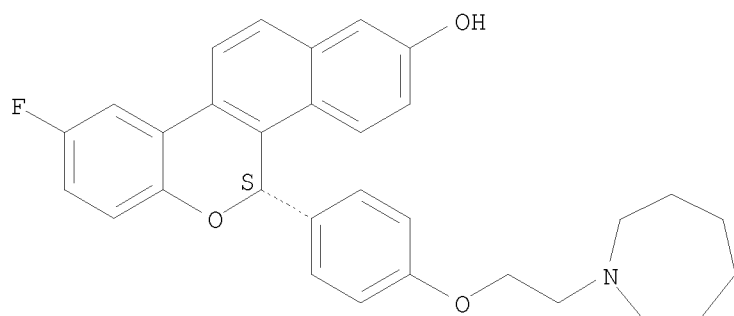
Absolute stereochemistry.



RN 861931-57-9 CAPLUS

CN 5H-Benzo[b]naphtho[2,1-d]pyran-2-ol,
9-fluoro-5-[4-[2-(hexahydro-1H-azepin-1-yl)ethoxy]phenyl]-, (5S)- (CA
INDEX NAME)

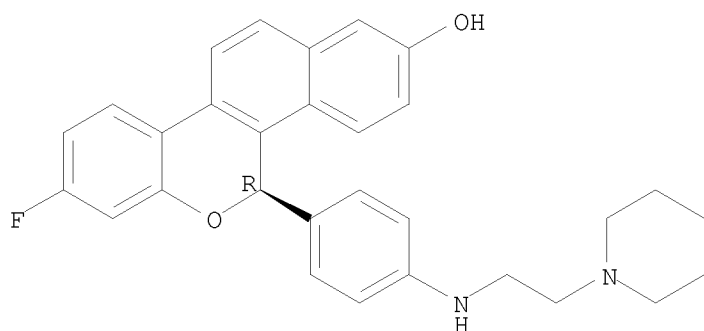
Absolute stereochemistry.



RN 861931-69-3 CAPLUS

CN 5H-Benzo[b]naphtho[2,1-d]pyran-2-ol,
8-fluoro-5-[4-[[2-(1-piperidinyl)ethyl]amino]phenyl]-, hydrochloride
(1:2), (5R)- (CA INDEX NAME)

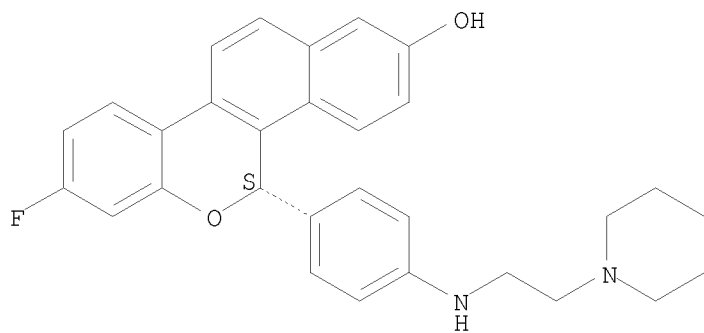
Absolute stereochemistry.



● 2 HCl

RN 861931-70-6 CAPLUS
 CN 5H-Benzo[b]naphtho[2,1-d]pyran-2-ol,
 8-fluoro-5-[4-[[2-(1-piperidinyl)ethyl]amino]phenyl]-, hydrochloride
 (1:2), (5S)- (CA INDEX NAME)

Absolute stereochemistry.



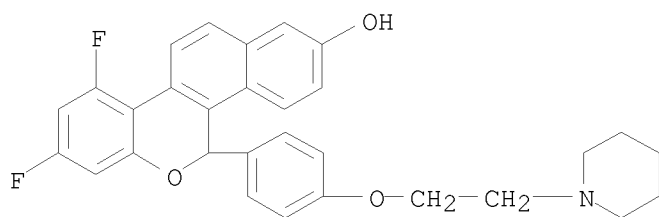
● 2 HCl

IT 861931-24-0P, 8,10-Difluoro-5-[4-[2-(piperidin-1-yl)ethoxy]phenyl]-5H-6-oxachrysen-2-ol 861931-29-5P,
 5-[4-[2-(Azepan-1-yl)ethoxy]phenyl]-7,10-difluoro-5H-6-oxachrysen-2-ol
 861931-31-9P, 7,10-Difluoro-5-[4-[2-(piperidin-1-yl)ethoxy]phenyl]-
 5H-6-oxachrysen-2-ol 861931-36-4P, Methanesulfonic acid
 7,9-difluoro-5-[4-[2-(piperidin-1-yl)ethoxy]phenyl]-5H-6-thiachrysen-2-yl
 ester 861931-40-0P, Methanesulfonic acid
 8-fluoro-5-[4-[2-(piperidin-1-yl)ethoxy]phenyl]-5H-6-thiachrysen-2-yl
 ester 861931-64-8P, 5-[4-[2-(Azepan-1-yl)ethoxy]phenyl]-8,10-
 difluoro-5H-6-oxachrysen-2-ol 861931-67-1P,
 [4-(8-Fluoro-2-methoxy-5H-6-oxachrysen-5-yl)phenyl][2-(piperidin-1-yl)ethyl]carbamic acid tert-butyl ester 861931-74-0P,
 1-[2-[4-(8-Fluoro-2-methoxy-5H-6-thiachrysen-5-yl)phenoxy]ethyl]piperidine

861931-81-9P, 2-Benzyloxy-8-fluoro-6-methyl-5-[4-[2-(piperidin-1-yl)ethoxy]phenyl]-5,6-dihydrobenzo[i]phenanthridine
 RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
 (drug candidate; preparation of piperidine derivs. as selective estrogen receptor modulators for treatment of vasomotor symptoms)

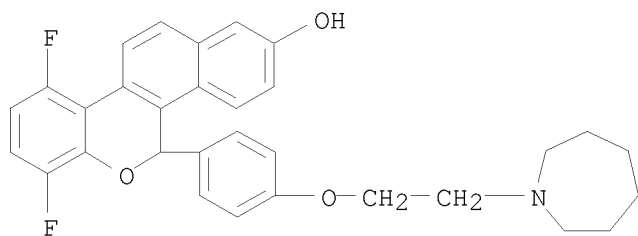
RN 861931-24-0 CAPLUS

CN 5H-Benzo[b]naphtho[2,1-d]pyran-2-ol,
 8,10-difluoro-5-[4-[2-(1-piperidinyloxy)phenyl]- (CA INDEX NAME)



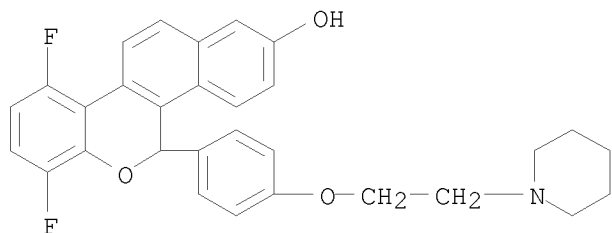
RN 861931-29-5 CAPLUS

CN 5H-Benzo[b]naphtho[2,1-d]pyran-2-ol,
 7,10-difluoro-5-[4-[2-(hexahydro-1H-azepin-1-yl)ethoxy]phenyl]- (CA INDEX NAME)



RN 861931-31-9 CAPLUS

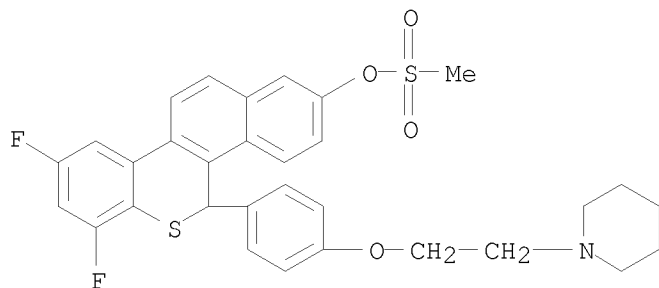
CN 5H-Benzo[b]naphtho[2,1-d]pyran-2-ol,
 7,10-difluoro-5-[4-[2-(1-piperidinyloxy)phenyl]- (CA INDEX NAME)



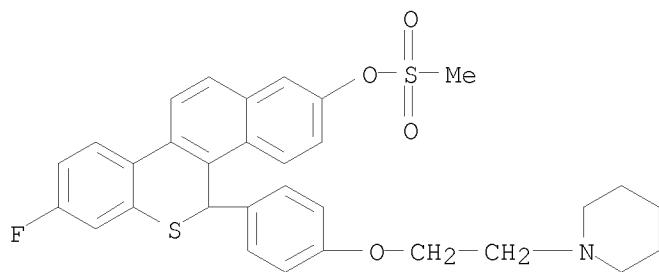
RN 861931-36-4 CAPLUS

CN 5H-Benzo[b]naphtho[2,1-d]thiopyran-2-ol,
 7,9-difluoro-5-[4-[2-(1-piperidinyloxy)phenyl]-, 2-methanesulfonate
 (CA INDEX NAME)

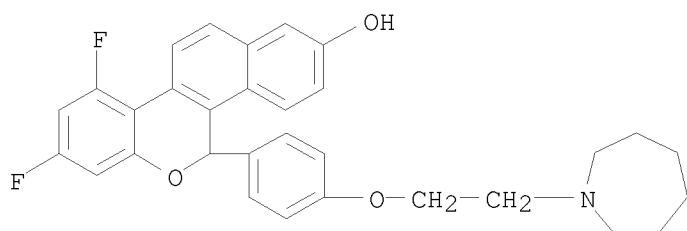
10/597,241



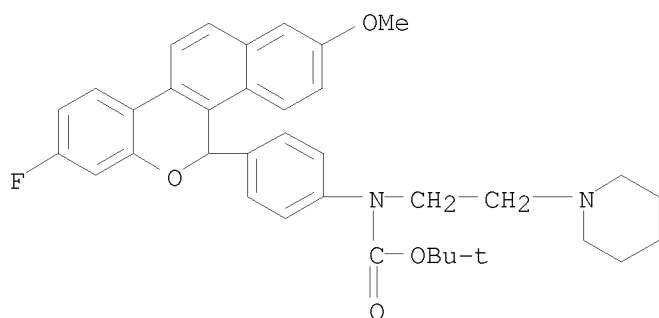
RN 861931-40-0 CAPLUS
CN 5H-Benzo[b]naphtho[2,1-d]thiopyran-2-ol,
8-fluoro-5-[4-[2-(1-piperidinyl)ethoxy]phenyl]-, 2-methanesulfonate (CA
INDEX NAME)



RN 861931-64-8 CAPLUS
CN 5H-Benzo[b]naphtho[2,1-d]pyran-2-ol,
8,10-difluoro-5-[4-[2-(hexahydro-1H-azepin-1-yl)ethoxy]phenyl]- (CA INDEX
NAME)

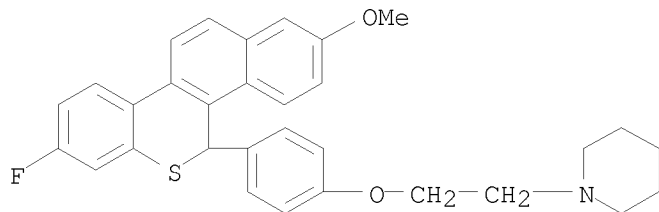


RN 861931-67-1 CAPLUS
CN Carbamic acid, [4-(8-fluoro-2-methoxy-5H-benzo[b]naphtho[2,1-d]pyran-5-
yl)phenyl][2-(1-piperidinyl)ethyl]-, 1,1-dimethylethyl ester (9CI) (CA
INDEX NAME)



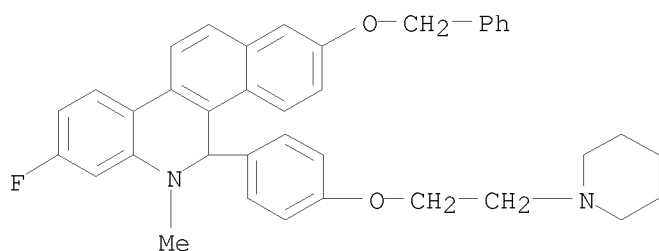
RN 861931-74-0 CAPLUS

CN Piperidine, 1-[2-[4-(8-fluoro-2-methoxy-5H-benzo[b]naphtho[2,1-d]thiopyran-5-yl)phenoxy]ethyl]- (CA INDEX NAME)



RN 861931-81-9 CAPLUS

CN Benzo[i]phenanthridine, 8-fluoro-5,6-dihydro-6-methyl-2-(phenylmethoxy)-5-[4-[2-(1-piperidinyl)ethoxy]phenyl]- (CA INDEX NAME)



IT 861931-22-8P, 7,9-Difluoro-5-[4-[2-(piperidin-1-yl)ethoxy]phenyl]-5H-6-oxachrysen-2-ol hydrochloride
 861931-28-4P, 5-[4-[2-(Azepan-1-yl)ethoxy]phenyl]-7,10-difluoro-5H-6-oxachrysen-2-ol hydrochloride 861931-30-8P,
 7,10-Difluoro-5-[4-[2-(piperidin-1-yl)ethoxy]phenyl]-5H-6-oxachrysen-2-ol hydrochloride 861931-37-5P,
 7,9-Difluoro-5-[4-[2-(piperidin-1-yl)ethoxy]phenyl]-5H-6-thiachrysen-2-ol hydrochloride 861931-41-1P,
 8-Fluoro-5-[4-[2-(piperidin-1-yl)ethoxy]phenyl]-5H-6-thiachrysen-2-ol hydrochloride 861931-44-4P,
 8-Fluoro-5-[4-[2-(piperidin-1-yl)ethoxy]phenyl]-5H-6-oxachrysen-2-ol 861931-45-5P, 10-Fluoro-5-[4-[2-(piperidin-1-yl)ethoxy]phenyl]-5H-

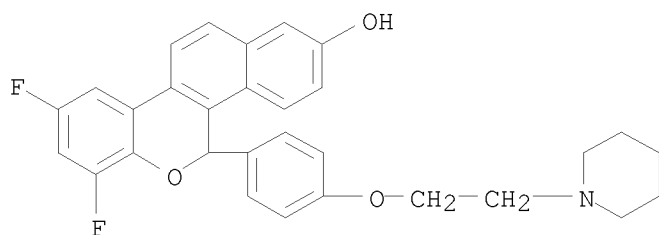
6-oxachrysen-2-ol 861931-53-5P,
 5-[4-[2-(Azepan-1-yl)ethoxy]phenyl]-8-fluoro-5H-6-oxachrysen-2-ol
 hydrochloride 861931-61-5P,
 5-[4-[2-(Azepan-1-yl)ethoxy]phenyl]-7,9-difluoro-5H-6-oxachrysen-2-ol
 861931-63-7P, 5-[4-[2-(Azepan-1-yl)ethoxy]phenyl]-8,10-difluoro-5H-
 6-oxachrysen-2-ol hydrochloride 861931-71-7P
 861931-78-4P, 8-Fluoro-5-[4-[2-(piperidin-1-yl)ethoxy]phenyl]-5,6-
 dihydrobenzo[i]phenanthridin-2-ol 861931-82-0P,
 8-Fluoro-6-methyl-5-[4-[2-(piperidin-1-yl)ethoxy]phenyl]-5,6-
 dihydrobenzo[i]phenanthridin-2-ol 861931-86-4P,
 5-[4-[2-(Piperidin-1-yl)ethoxy]phenyl]-8,9-difluoro-5H-6-oxachrysen-2-ol
 hydrochloride

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
 (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES

(Uses)
 (drug candidate; preparation of piperidine derivs. as selective estrogen
 receptor modulators for treatment of vasomotor symptoms)

RN 861931-22-8 CAPLUS

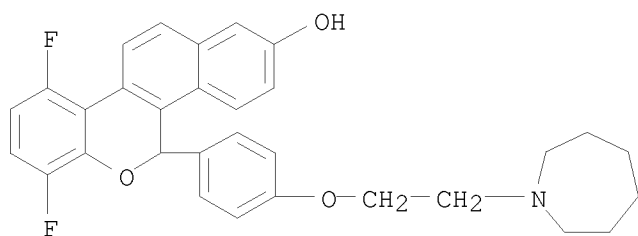
CN 5H-Benzo[b]naphtho[2,1-d]pyran-2-ol,
 7,9-difluoro-5-[4-[2-(1-piperidinyl)ethoxy]phenyl]-, hydrochloride (1:1)
 (CA INDEX NAME)



● HCl

RN 861931-28-4 CAPLUS

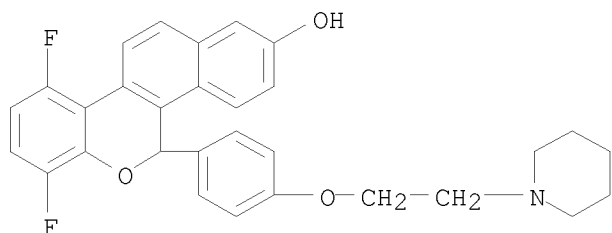
CN 5H-Benzo[b]naphtho[2,1-d]pyran-2-ol,
 7,10-difluoro-5-[4-[2-(hexahydro-1H-azepin-1-yl)ethoxy]phenyl]-,
 hydrochloride (1:1) (CA INDEX NAME)



● HCl

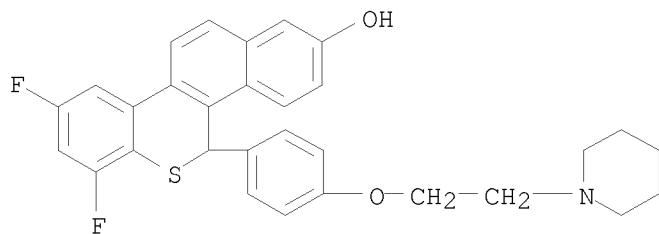
10/597,241

RN 861931-30-8 CAPLUS
CN 5H-Benzo[b]naphtho[2,1-d]pyran-2-ol,
7,10-difluoro-5-[4-[2-(1-piperidinyl)ethoxy]phenyl]-, hydrochloride (1:1)
(CA INDEX NAME)



● HCl

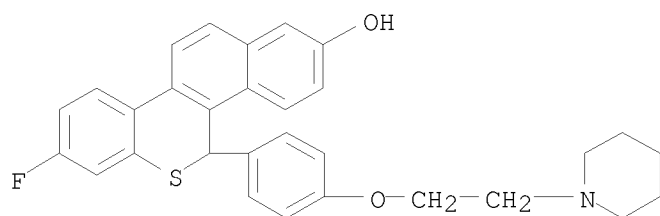
RN 861931-37-5 CAPLUS
CN 5H-Benzo[b]naphtho[2,1-d]thiopyran-2-ol,
7,9-difluoro-5-[4-[2-(1-piperidinyl)ethoxy]phenyl]-, hydrochloride (1:1)
(CA INDEX NAME)



● HCl

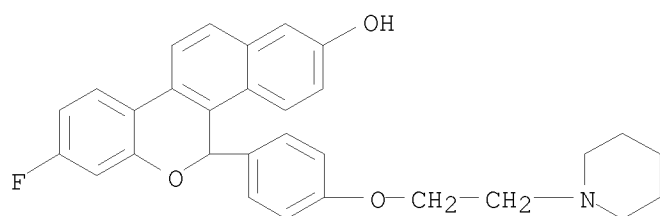
RN 861931-41-1 CAPLUS
CN 5H-Benzo[b]naphtho[2,1-d]thiopyran-2-ol,
8-fluoro-5-[4-[2-(1-piperidinyl)ethoxy]phenyl]-, hydrochloride (1:1) (CA
INDEX NAME)

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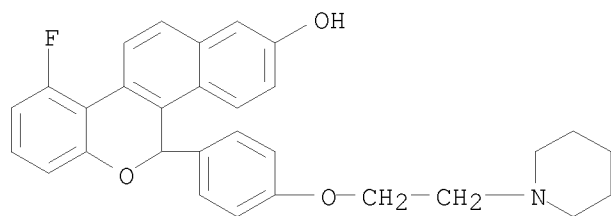


● HCl

RN 861931-44-4 CAPLUS
CN 5H-Benzo[b]naphtho[2,1-d]pyran-2-ol,
8-fluoro-5-[4-[2-(1-piperidinyl)ethoxy]phenyl]- (CA INDEX NAME)

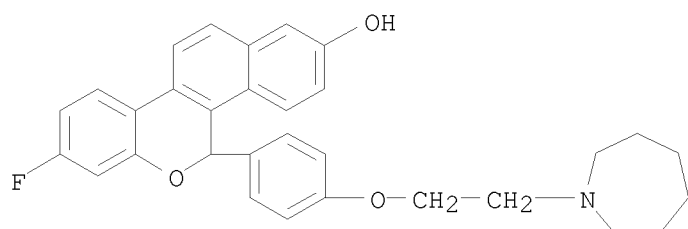


RN 861931-45-5 CAPLUS
CN 5H-Benzo[b]naphtho[2,1-d]pyran-2-ol,
10-fluoro-5-[4-[2-(1-piperidinyl)ethoxy]phenyl]- (CA INDEX NAME)



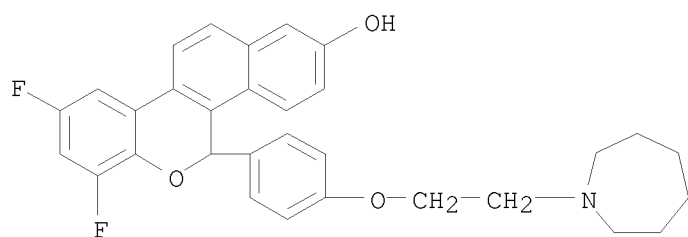
RN 861931-53-5 CAPLUS
CN 5H-Benzo[b]naphtho[2,1-d]pyran-2-ol,
8-fluoro-5-[4-[2-(hexahydro-1H-azepin-1-yl)ethoxy]phenyl]-, hydrochloride
(1:1) (CA INDEX NAME)

10/597,241

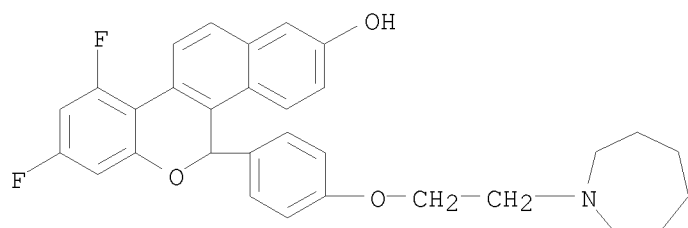


● HCl

RN 861931-61-5 CAPLUS
CN 5H-Benzo[b]naphtho[2,1-d]pyran-2-ol,
7,9-difluoro-5-[4-[2-(hexahydro-1H-azepin-1-yl)ethoxy]phenyl]- (CA INDEX
NAME)



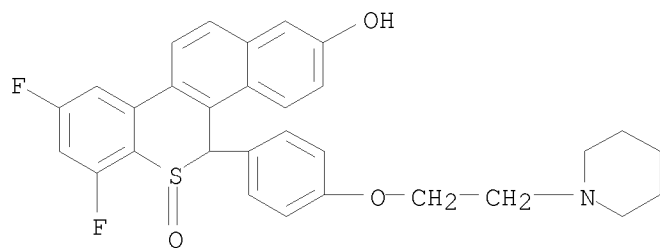
RN 861931-63-7 CAPLUS
CN 5H-Benzo[b]naphtho[2,1-d]pyran-2-ol,
8,10-difluoro-5-[4-[2-(hexahydro-1H-azepin-1-yl)ethoxy]phenyl]-,
hydrochloride (1:1) (CA INDEX NAME)



● HCl

RN 861931-71-7 CAPLUS
CN 5H-Benzo[b]naphtho[2,1-d]thiopyran-2-ol,
7,9-difluoro-5-[4-[2-(1-piperidinyl)ethoxy]phenyl]-, 6-oxide,
hydrochloride (1:1) (CA INDEX NAME)

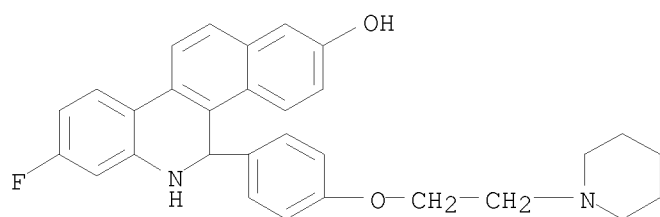
10/597,241



● HCl

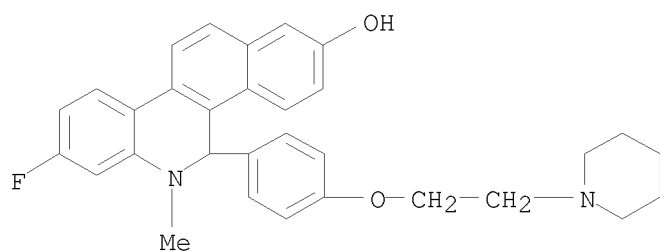
RN 861931-78-4 CAPLUS

CN Benzo[i]phenanthridin-2-ol, 8-fluoro-5,6-dihydro-5-[4-[2-(1-piperidinyl)ethoxy]phenyl]- (CA INDEX NAME)



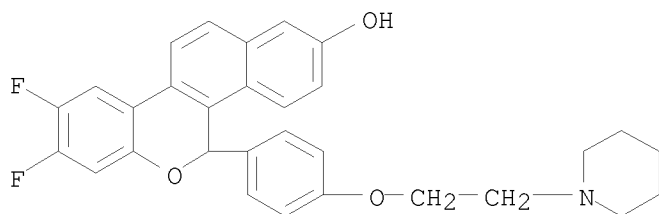
RN 861931-82-0 CAPLUS

CN Benzo[i]phenanthridin-2-ol, 8-fluoro-5,6-dihydro-6-methyl-5-[4-[2-(1-piperidinyl)ethoxy]phenyl]- (CA INDEX NAME)



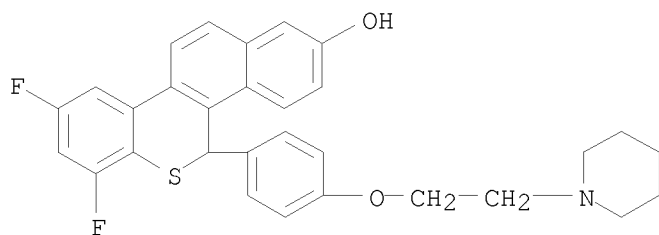
RN 861931-86-4 CAPLUS

CN 5H-Benzo[b]naphtho[2,1-d]pyran-2-ol, 8,9-difluoro-5-[4-[2-(1-piperidinyl)ethoxy]phenyl]-, hydrochloride (1:1) (CA INDEX NAME)

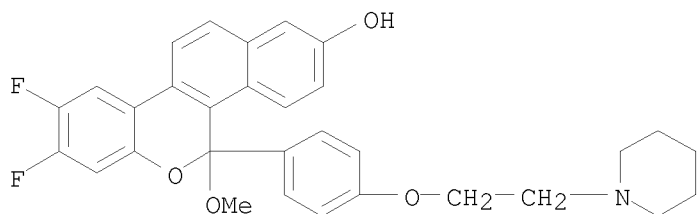


● HCl

IT 861931-72-8, 7,9-Difluoro-5-[4-[2-(piperidin-1-yl)ethoxy]phenyl]-
5H-6-thiachrysen-2-ol
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of piperidine derivs. as selective estrogen receptor modulators
for treatment of vasomotor symptoms)
RN 861931-72-8 CAPLUS
CN 5H-Benzo[b]naphtho[2,1-d]thiopyran-2-ol,
7,9-difluoro-5-[4-[2-(1-piperidinyl)ethoxy]phenyl]- (CA INDEX NAME)



IT 861931-84-2P, 8,9-Difluoro-5-methoxy-5-[4-[2-(piperidin-1-yl)ethoxy]phenyl]-5H-6-oxachrysen-2-ol
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)
(preparation of piperidine derivs. as selective estrogen receptor modulators
for treatment of vasomotor symptoms)
RN 861931-84-2 CAPLUS
CN 5H-Benzo[b]naphtho[2,1-d]pyran-2-ol,
8,9-difluoro-5-methoxy-5-[4-[2-(1-piperidinyl)ethoxy]phenyl]- (CA INDEX
NAME)



10/597,241

OS.CITING REF COUNT:	1	THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD (1 CITINGS)
REFERENCE COUNT:	7	THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 5 OF 15 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2005:478998 CAPLUS

DOCUMENT NUMBER: 143:165982

TITLE: A pharmacophore-based evolutionary approach for screening selective estrogen receptor modulators

AUTHOR(S): Yang, Jinn-Moon; Shen, Tsai-Wei

CORPORATE SOURCE: Department of Biological Science and Technology, National Chiao Tung University, Hsinchu, Taiwan

SOURCE: Proteins: Structure, Function, and Bioinformatics (2005), 59(2), 205-220

CODEN: PSFBAF

PUBLISHER: Wiley-Liss, Inc.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The authors developed a pharmacophore-based evolutionary approach for virtual screening. This tool, termed the Generic Evolutionary Method for mol. DOCKing (GEMDOCK), combines an evolutionary approach with a new pharmacophore-based scoring function. The former integrates discrete and continuous global search strategies with local search strategies to expedite convergence. The latter, integrating an empirical-based energy function and pharmacol. preferences (binding-site pharmacol. interactions and ligand preferences), simultaneously serves as the scoring function for both mol. docking and postdocking analyses to improve screening accuracy. The authors apply pharmacol. interaction preferences to select the ligands that form pharmacol. interactions with target proteins, and use the ligand preferences to eliminate the ligands that violate the electrostatic or hydrophilic constraints. The authors assessed the accuracy of our approach using human estrogen receptor (ER) and a ligand database from the comparative studies of Bissantz et al. (J Med Chem 2000;43:4759-4767). Using GEMDOCK, the average goodness-of-hit (GH) score was 0.83 and the average false-pos. rate was 0.13% for ER antagonists, and the average GH score was 0.48 and the average false-pos. rate was 0.75% for ER agonists. The performance of GEMDOCK was superior to competing methods such as GOLD and DOCK. The authors found that our pharmacophore-based scoring function indeed was able to reduce the number of false positives; moreover, the resulting pharmacol. interactions at the binding site, as well as ligand preferences, were important to the screening accuracy of our expts. These results suggest that GEMDOCK constitutes a robust tool for virtual database screening.

IT 188824-17-1, LY-357489

RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL

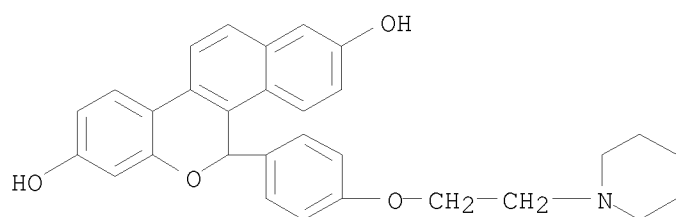
(Biological study); USES (Uses)

(pharmacophore-based evolutionary approach for screening selective estrogen receptor modulators)

RN 188824-17-1 CAPLUS

CN 5H-Benzo[b]naphtho[2,1-d]pyran-2,8-diol,
5-[4-[2-(1-piperidinyl)ethoxy]phenyl]- (CA INDEX NAME)

10/597,241



OS.CITING REF COUNT:	27	THERE ARE 27 CAPLUS RECORDS THAT CITE THIS RECORD (28 CITINGS)
REFERENCE COUNT:	35	THERE ARE 35 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 6 OF 15 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2004:548950 CAPLUS

DOCUMENT NUMBER: 141:134250

TITLE: Is it possible docking and scoring new ligands with few experimental data? Preliminary results on estrogen receptor as a case study

AUTHOR(S): Cozzini, P.; Dottorini, T.

CORPORATE SOURCE: Molecular Modelling Laboratory, Department of General and Inorganic Chemistry, Parco Area delle Scienze, University of Parma, Parma, 43100, Italy

SOURCE: European Journal of Medicinal Chemistry (2004), 39(7), 601-609

CODEN: EJMCA5; ISSN: 0223-5234

PUBLISHER: Elsevier Science Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

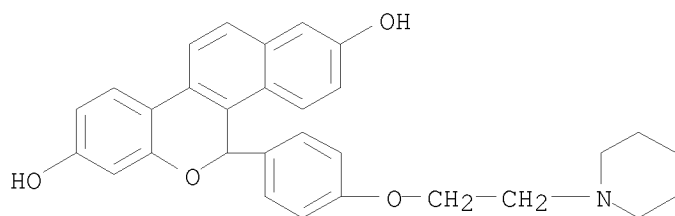
AB Estrogens are steroid hormones playing critical roles in several physiol. processes, which bind the estrogen receptors ER α and ER β . Aim of this work is to analyze, by different docking expts., the behavior of a set of compds., mimicking estrogens activity, to understand the relationship between ER α and such new ligands. Main goal is to verify, using a widely tested scoring software procedure applied on a set of 10 compds., the possibility to produce new lead candidate mols. in lack of, or with few exptl. data. The authors' preliminary results reveal the significance of HINT software as a scoring function in docking methodol. and specifically, as a mean for assessing the consistency of docking solns.

IT 188824-17-1

RL: BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study)

(possible docking and scoring new ligands with few exptl. data in relation to preliminary results on estrogen receptor)

RN 188824-17-1 CAPLUS

CN 5H-Benzo[b]naphtho[2,1-d]pyran-2,8-diol,
5-[4-[2-(1-piperidinyl)ethoxy]phenyl]- (CA INDEX NAME)

OS.CITING REF COUNT: 5 THERE ARE 5 CAPLUS RECORDS THAT CITE THIS RECORD (5 CITINGS)

REFERENCE COUNT: 27 THERE ARE 27 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 7 OF 15 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2004:42543 CAPLUS

DOCUMENT NUMBER: 140:246121

TITLE: Ligand-Based Structural Hypotheses for Virtual Screening

AUTHOR(S): Jain, Ajay N.

CORPORATE SOURCE: UCSF Cancer Research Institute and Comprehensive Cancer Center, University of California, San Francisco, CA, 94143-0128, USA

SOURCE: Journal of Medicinal Chemistry (2004), 47(4), 947-961
CODEN: JMCMAR; ISSN: 0022-2623

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The majority of drug targets for small mol. therapeutics are proteins whose three-dimensional structure is not known to sufficient resolution to permit structure-based design. All three-dimensional QSAR approaches have a requirement for some hypothesis of ligand conformation and alignment, and predictions of mol. activity critically depend on this ligand-based binding site hypothesis. The mol. similarity function used in the Surflex docking system, coupled with quant. pressure to minimize overall mol. volume, forms an effective objective function for generating hypotheses of bioactive conformations of sets of small mols. binding to their cognate proteins. Results are presented, assessing utility of the method for ligands of the serotonin, histamine, muscarinic, and GABAA receptors. The Surflex similarity module (Surflex-Sim) was able, in each case, to distinguish true ligands from random compds. using models constructed from just two or three known ligands. True pos. rates of 60% were achieved with false pos. rates of 0-3%; the theor. enrichment rates were over 150-fold compared with random screening. The methods are practically applicable for rational design of ligands and for high-throughput virtual screening and offer competitive performance to many structure-based docking algorithms.

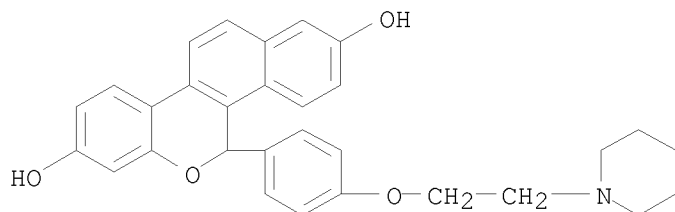
IT 188824-17-1, LY-357489

RL: PAC (Pharmacological activity); PRP (Properties); BIOL (Biological study)

(estrogen receptor ligand; ligand-based structural hypotheses for virtual screening applied to ligands of different receptors and targets)

RN 188824-17-1 CAPLUS

CN 5H-Benzo[b]naphtho[2,1-d]pyran-2,8-diol,
5-[4-[2-(1-piperidinyloxy)ethoxy]phenyl]- (CA INDEX NAME)



OS.CITING REF COUNT: 38 THERE ARE 38 CAPLUS RECORDS THAT CITE THIS
RECORD (38 CITINGS)

REFERENCE COUNT: 31 THERE ARE 31 CITED REFERENCES AVAILABLE FOR THIS

10/597,241

RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 8 OF 15 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2003:678670 CAPLUS

DOCUMENT NUMBER: 139:192008

TITLE: Methods and composition for treating decreased libido
in women with estrogenic components

INVENTOR(S): Coelingh Bennink, Herman Jian Tijmen

PATENT ASSIGNEE(S): Pantarhei Bioscience B.V., Neth.

SOURCE: PCT Int. Appl., 17 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

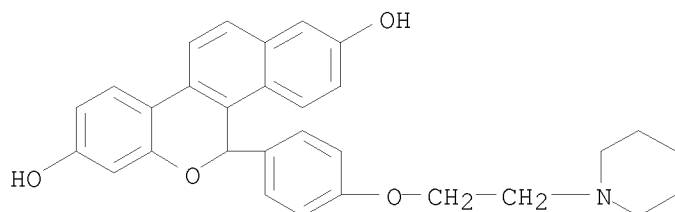
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003070253	A1	20030828	WO 2003-NL125	20030219
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW			
RW:	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
AU 2003206442	A1	20030909	AU 2003-206442	20030219
PRIORITY APPLN. INFO.:			EP 2002-75696	A 20020221
			WO 2003-NL125	W 20030219

AB The present invention is concerned with a method of treating decreased libido in pre-menopausal women, said decreased libido being the result of the repeated administration of a progestogenic component, wherein the method comprises the administration of the estrogenic component to a woman in an effective amount to improve the woman's libido. The present method is particularly suited for treating decreased libido in women using hormonal contraceptives that employ administration of a progestogenic component.

IT 188824-17-1, LY-357489

RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL
(Biological study); USES (Uses)(methods and composition for treating decreased libido in women with
estrogenic components)

RN 188824-17-1 CAPLUS

CN 5H-Benzo[b]naphtho[2,1-d]pyran-2,8-diol,
5-[4-[2-(1-piperidinyl)ethoxy]phenyl]- (CA INDEX NAME)

10/597,241

REFERENCE COUNT:

9

THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 9 OF 15 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2003:498000 CAPLUS

DOCUMENT NUMBER: 139:176251

TITLE: BHB: A simple knowledge-based scoring function to improve the efficiency of database screening

AUTHOR(S): Feher, Miklos; Deretey, Eugen; Roy, Samir

CORPORATE SOURCE: SignalGene Inc., Guelph, ON, N1G 4P7, Can.

SOURCE: Journal of Chemical Information and Computer Sciences (2003), 43(4), 1316-1327

CODEN: JCISD8; ISSN: 0095-2338

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

AB A new knowledge-based scoring function was developed in this work to facilitate the rapid ranking of ligands in databases. The acronym of the method is BHB based on the descriptors it utilizes: buriedness, hydrogen bonding, and binding energy. Receptor buriedness is a measure of how well mols. occupy the binding pocket in comparison to known high-affinity ligands or, alternatively, whether they have contact with identified residues in the pocket. The possibility of hydrogen bond formation is checked for selected residues that are recognized as being important in the binding of known ligands. The approx. binding energy is calculated from the thermodyn. cycle using the optimized bound and free solvent conformations of the ligand-receptor system. The information necessary for the scoring function can ideally be gleaned from the 3D structure of the receptor-ligand complex. Alternatively, the descriptors can be derived from the 3D structure of the unbound receptor, provided this receptor has a known ligand that binds to the given site with nanomolar activity. We show that the new scoring functions provide up to 12 times improvement in enrichment compared to the popular com. docking program GOLD.

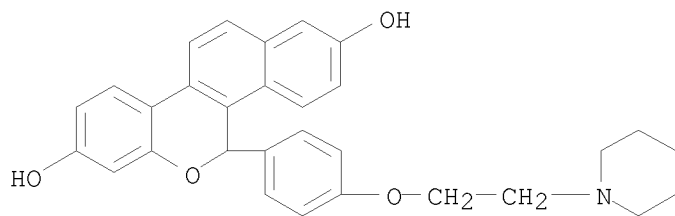
IT 188824-17-1, LY-357489

RL: BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study)

(BHB knowledge-based scoring function to improve the efficiency of database screening)

RN 188824-17-1 CAPLUS

CN 5H-Benzo[b]naphtho[2,1-d]pyran-2,8-diol,
5-[4-[2-(1-piperidinyl)ethoxy]phenyl]- (CA INDEX NAME)



OS.CITING REF COUNT: 15 THERE ARE 15 CAPLUS RECORDS THAT CITE THIS RECORD (15 CITINGS)

REFERENCE COUNT: 50 THERE ARE 50 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 10 OF 15 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2002:940242 CAPLUS

DOCUMENT NUMBER: 137:380017

TITLE: Estrogen receptor β -based hypertension treatment and assay

INVENTOR(S): Gustafsson, Jan-Ake; Bian, Zhao

PATENT ASSIGNEE(S): Karo Bio AB, Swed.

SOURCE: Brit. UK Pat. Appl., 28 pp.

CODEN: BAXXDU

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

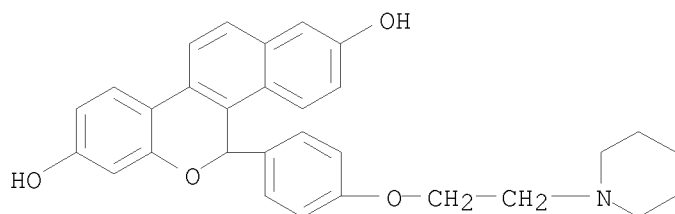
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
GB 2374412	A	20021016	GB 2001-9091	20010411
PRIORITY APPLN. INFO.:			GB 2001-9091	20010411

AB Methods are disclosed for assaying compds. for blood pressure-modulating activity. The methods include determining the ability of the compound to affect estrogen receptor β (ER β) activity. The invention also discloses the use of ER β -modulating compds. for modulating blood pressure, in particular for treating hypertension.

IT 188824-17-1, LY-357489
 RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
 (estrogen receptor β -based hypertension treatment and assay)

RN 188824-17-1 CAPLUS

CN 5H-Benzo[b]naphtho[2,1-d]pyran-2,8-diol,
 5-[4-[2-(1-piperidinyloxy)phenyl]- (CA INDEX NAME)



OS.CITING REF COUNT: 2 THERE ARE 2 CAPLUS RECORDS THAT CITE THIS RECORD (2 CITINGS)

L11 ANSWER 11 OF 15 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2002:210373 CAPLUS

DOCUMENT NUMBER: 137:87830

TITLE: Molecular simulation of interaction between estrogen receptor and selective estrogen receptor modulators

AUTHOR(S): Guo, Zong-Ru; Yi, Xiang; Xu, Zhi-Bin

CORPORATE SOURCE: Institute of Materia Medica, Chinese Academy of Medical Sciences and Peking Union Medical College, Beijing, 100050, Peop. Rep. China

SOURCE: Acta Pharmacologica Sinica (2002), 23(3), 208-212
CODEN: APSCG5; ISSN: 1671-4083

PUBLISHER: Science Press

DOCUMENT TYPE: Journal

LANGUAGE: English

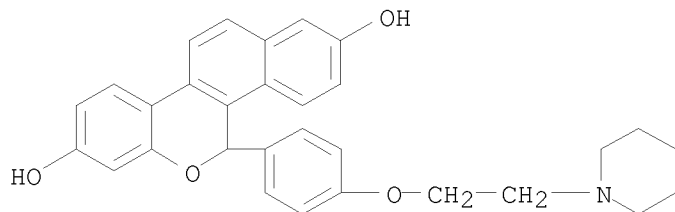
AB Aim: To study the mechanism of interaction between a series of potent racemic selective estrogen receptor modulators (SERM) and estrogen receptors (ER). Methods: Active conformations of these conformationally restricted raloxifene analogs in binding pocket were determined by mol. mechanics. The interactive energies between ligand and receptor were calculated by docking program. Results: Both R and S configurations of these SERM were accommodated by the binding pocket of ER. The hydroxy group of compds. forms hydrogen bonds with amino acid residues of ER and the phenolic group mimics the A-ring of estradiol. The most potential compds. were those with two hydroxy groups and accommodated by binding pocket in S configuration with phenolic group at C(16) imitating A-ring of estradiol. Conclusion: Chiral center conferred little effect on the binding affinity of these conformationally restricted raloxifene analogs. The hydroxy group(s) play(s) a critical role to the orientation of compds. in active pocket of ER and the binding between ligand and receptor.

IT 188824-17-1

RL: PAC (Pharmacological activity); PRP (Properties); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(mol. simulation of estrogen receptor interaction with estrogen receptor modulators)

RN 188824-17-1 CAPLUS

CN 5H-Benzo[b]naphtho[2,1-d]pyran-2,8-diol,
5-[4-[2-(1-piperidinyl)ethoxy]phenyl]- (CA INDEX NAME)

OS.CITING REF COUNT: 2 THERE ARE 2 CAPLUS RECORDS THAT CITE THIS RECORD (2 CITINGS)

REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 12 OF 15 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2000:818588 CAPLUS

DOCUMENT NUMBER: 134:125545

TITLE: Protein-Based Virtual Screening of Chemical Databases.
1. Evaluation of Different Docking/Scoring
Combinations

AUTHOR(S): Bissantz, Caterina; Folkers, Gerd; Rognan, Didier

CORPORATE SOURCE: Department of Applied Biosciences, ETH Zuerich,
Zurich, CH-8057, Switz.SOURCE: Journal of Medicinal Chemistry (2000), 43(25),
4759-4767

CODEN: JMCMAR; ISSN: 0022-2623

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

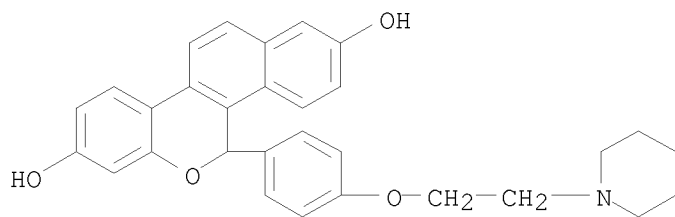
AB Three different database docking programs (Dock, FlexX, Gold) have been used in combination with seven scoring functions (Chemscore, Dock, FlexX, Fresno, Gold, Pmf, Score) to assess the accuracy of virtual screening methods against two protein targets (thymidine kinase, estrogen receptor) of known three-dimensional structure. For both targets, it was generally possible to discriminate about 7 out of 10 true hits from a random database of 990 ligands. The use of consensus lists common to two or three scoring functions clearly enhances hit rates among the top 5% scorers from 10% (single scoring) to 25-40% (double scoring) and up to 65-70% (triple scoring). However, in all tested cases, no clear relationships could be found between docking and ranking accuracies. Moreover, predicting the absolute binding free energy of true hits was not possible whatever docking accuracy was achieved and scoring function used. As the best docking/consensus scoring combination varies with the selected target and the physicochem. of target-ligand interactions, we propose a two-step protocol for screening large databases: (i) screening of a reduced dataset containing a few known ligands for deriving the optimal docking/consensus scoring scheme, (ii) applying the latter parameters to the screening of the entire database.

IT 188824-17-1, LY 357489

RL: PRP (Properties)

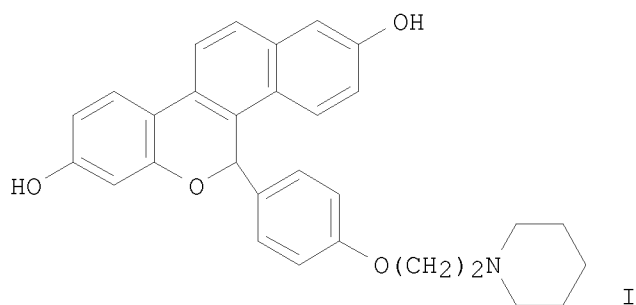
(accuracy of virtual screening methods against protein targets of known structure)

RN 188824-17-1 CAPLUS

CN 5H-Benzo[b]naphtho[2,1-d]pyran-2,8-diol,
5-[4-[2-(1-piperidinyl)ethoxy]phenyl]- (CA INDEX NAME)OS.CITING REF COUNT: 383 THERE ARE 383 CAPLUS RECORDS THAT CITE THIS
RECORD (384 CITINGS)REFERENCE COUNT: 50 THERE ARE 50 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 13 OF 15 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1998:215077 CAPLUS
 DOCUMENT NUMBER: 128:266187
 ORIGINAL REFERENCE NO.: 128:52547a,52550a
 TITLE: Synthesis and Pharmacology of Conformationally
 Restricted Raloxifene Analogs: Highly Potent Selective
 Estrogen Receptor Modulators
 AUTHOR(S): Grese, Timothy A.; Pennington, Lewis D.; Sluka, James
 P.; Adrian, M. Dee; Cole, Harlan W.; Fuson, Tina R.;
 Magee, David E.; Phillips, D. Lynn; Rowley, Ellen R.;
 Shetler, Pamela K.; Short, Lorri L.; Venugopalan,
 Murali; Yang, Na N.; Sato, Masahiko; Glasebrook,
 Andrew L.; Bryant, Henry U.
 CORPORATE SOURCE: Lilly Research Laboratories, Eli Lilly and Company,
 Indianapolis, IN, 46285, USA
 SOURCE: Journal of Medicinal Chemistry (1998), 41(8),
 1272-1283
 CODEN: JMCMAR; ISSN: 0022-2623
 PUBLISHER: American Chemical Society
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI



AB Raloxifene is a selective estrogen receptor modulator (SERM) which is currently under clin. evaluation for the prevention and treatment of postmenopausal osteoporosis. In vivo structure-activity relationships and mol. modeling studies indicated that the orientation of the basic amine-containing side chain of raloxifene relative to the stilbene plane is an important discriminating factor for the maintenance of tissue selectivity. A series of raloxifene analogs where this side chain is held in an orientation which is orthogonal to the stilbene plane, similar to the low-energy conformation predicted for raloxifene were constructed. These analogs were prepared and tested for their activity in a series of in vitro and in vivo biol. assays reflective of the SERM profile. The ability of these analogs to (1) bind the estrogen receptor, (2) antagonize estrogen-stimulated proliferation of MCF-7 cells in vitro, (3) stimulate TGF- β 3 gene expression in cell culture, (4) inhibit the uterine effects of ethynyl estradiol in immature rats, and (5) potentially reduce serum cholesterol and protect against osteopenia in ovariectomized (OVX) rats without estrogen-like stimulation of uterine tissue is detailed. These data demonstrate that LY357489 (I) is among the most potent SERMs described to date with in vivo efficacy on bone and cholesterol metabolism in

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OVX rats at doses as low as 0.01 mg/kg/d.

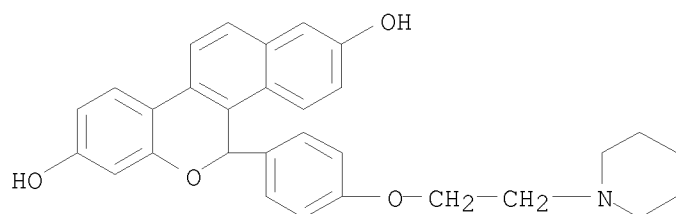
IT 188824-17-1P, LY 357489

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(preparation of conformationally restricted raloxifene analogs and pharmacol. as selective estrogen receptor modulators)

RN 188824-17-1 CAPLUS

CN 5H-Benzo[b]naphtho[2,1-d]pyran-2,8-diol,
5-[4-[2-(1-piperidinyloxy)phenyl]- (CA INDEX NAME)

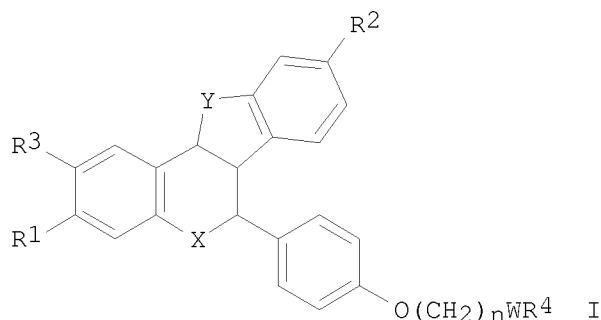


OS.CITING REF COUNT: 92 THERE ARE 92 CAPLUS RECORDS THAT CITE THIS
RECORD (92 CITINGS)
REFERENCE COUNT: 60 THERE ARE 60 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 14 OF 15 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1998:180547 CAPLUS
 DOCUMENT NUMBER: 128:217362
 ORIGINAL REFERENCE NO.: 128:43059a, 43062a
 TITLE: Preparation of benzothienobenzopyrans,
 benzophenanthridines, and related compounds for
 treatment of postmenopausal syndrome.
 INVENTOR(S): Grese, Timothy Alan
 PATENT ASSIGNEE(S): Eli Lilly and Co., USA
 SOURCE: U.S., 39 pp.
 CODEN: USXXAM
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 2
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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US 5726186	A	19980310	US 1996-696279	19960813
US 6004971	A	19991221	US 1997-878799	19970619
US 6133288	A	20001017	US 1999-436743	19991109
PRIORITY APPLN. INFO.:			US 1995-3496P	P 19950908
			US 1996-696279	A3 19960813
			US 1997-878799	A1 19970619
OTHER SOURCE(S):	MARPAT 128:217362			
GI				

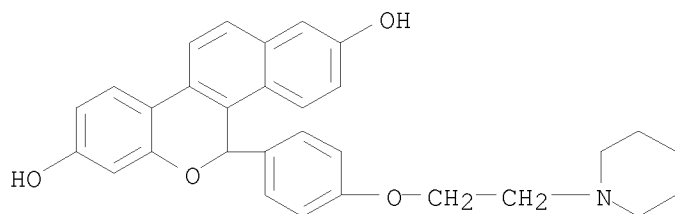


AB Title compds. [I; X = O, S; Y = O, S, CH₂, CH₂CH₂, CH:CH, NR₅; R₁-R₃ = H, OH, alkoxy, PhCO₂, alkylcarbonyloxy, alkylsulfonyloxy, OSO₂CF₃, Cl, F; n = 1, 2; W = CH₂, CO; R₄ = 1-piperidinyl, 2-oxo-1-piperidinyl, 1-pyrrolidinyl, methyl-1-pyrrolidinyl, dimethyl-1-pyrrolidinyl, 2-oxo-1-pyrrolidinyl, 4-morpholino, dimethylamino, diethylamino, 1-hexamethyleneimino; R₅ = alkyl, PhCO, alkylcarbonyl, phenoxy carbonyl, alkoxy carbonyl, alkylsulfonyl, phenylsulfonyl, SO₂CF₃], were prepared Thus, 6-methoxythianaphthalen-2-one (preparation given) was stirred with 4-methoxysalicylaldehyde and Et₃N in CH₂Cl₂ to give 6a,11a-dihydro-3,9-dimethoxy-6H-[1]benzothieno[3,2-c][1]benzopyran-6-one. This was converted in several steps to 3,9-dihydroxy-6-[4-[2-(1-piperidinyl)ethoxy]phenyl]-6H-[1]benzothieno[3,2-c][1]benzopyran. The latter at 0.1 mg/kg in ovariectomized rats reduced serum cholesterol by 72.8%.
 IT 188824-17-1P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
 (preparation of benzothienobenzopyrans, benzophenanthridines, and related compds. for treatment of postmenopausal syndrome)

RN 188824-17-1 CAPLUS

CN 5H-Benzo[b]naphtho[2,1-d]pyran-2,8-diol,
 5-[4-[2-(1-piperidinyl)ethoxy]phenyl]- (CA INDEX NAME)



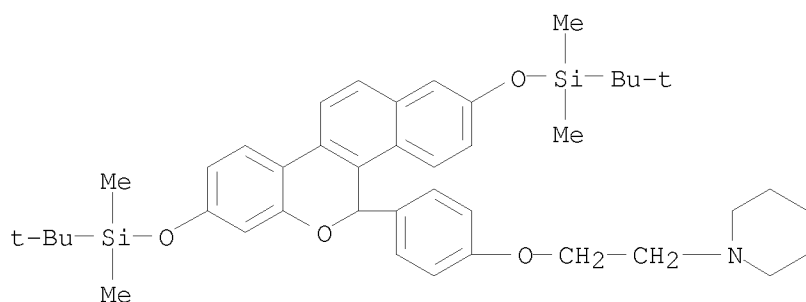
IT 188824-52-4P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of benzothienobenzopyrans, benzophenanthridines, and related compds. for treatment of postmenopausal syndrome)

RN 188824-52-4 CAPLUS

CN Piperidine, 1-[2-[4-[2,8-bis[[1,1-dimethylethyl]dimethylsilyl]oxy]-5H-benzo[b]naphtho[2,1-d]pyran-5-yl]phenoxy]ethyl]- (CA INDEX NAME)



OS.CITING REF COUNT: 3 THERE ARE 3 CAPLUS RECORDS THAT CITE THIS RECORD (5 CITINGS)

REFERENCE COUNT: 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 15 OF 15 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1997:286346 CAPLUS
 DOCUMENT NUMBER: 126:264018
 ORIGINAL REFERENCE NO.: 126:51137a,51140a
 TITLE: Preparation of pentacyclic compounds for the treatment conditions associated with post-menopausal syndrome
 INVENTOR(S): Grese, Timothy Alan
 PATENT ASSIGNEE(S): Eli Lilly and Co., USA
 SOURCE: Eur. Pat. Appl., 72 pp.
 CODEN: EPXXDW
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 2
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 761669	A2	19970312	EP 1996-306351	19960902
EP 761669	A3	19971029		
EP 761669	B1	20001122		
R: AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LI, LU, NL, PT, SE				
CA 2230974	A1	19970313	CA 1996-2230974	19960826
WO 9709044	A1	19970313	WO 1996-US13778	19960826
W: AL, AM, AU, AZ, BB, BG, BR, BY, CA, CN, CU, CZ, EE, GE, HU, IL, IS, JP, KE, KG, KP, KR, KZ, LK, LR, LS, LT, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, RO, RU, SD, SG, SI, SK, TJ, TM, TR, TT, UA, UG, US, UZ, VN				
RW: KE, LS, MW, SD, SZ, UG, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
AU 9669590	A	19970327	AU 1996-69590	19960826
AU 705454	B2	19990520		
CN 1201392	A	19981209	CN 1996-198083	19960826
HU 9802213	A2	19990201	HU 1998-2213	19960826
HU 9802213	A3	20000328		
BR 9610356	A	19990706	BR 1996-10356	19960826
JP 11514347	T	19991207	JP 1997-511257	19960826
JP 3688299	B2	20050824		
CZ 286236	B6	20000216	CZ 1998-678	19960826
IL 123560	A	20020210	IL 1996-123560	19960826
IL 140162	A	20020210	IL 1996-140162	19960826
AT 197712	T	20001215	AT 1996-306351	19960902
NO 9800936	A	19980507	NO 1998-936	19980304
GR 3035253	T3	20010430	GR 2001-400073	20010117
PRIORITY APPLN. INFO.:			US 1995-3496P	P 19950908
			IL 1996-123560	A3 19960826
			WO 1996-US13778	W 19960826
OTHER SOURCE(S):	MARPAT 126:264018			
GI				

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The title compds. [I and II; X = O, S, NR5 (wherein R5 = C1-3 alkyl, COPh, SO2CF3, etc.); Y = O, S, CH2, CH2CH2, CH:CH, NR5; B = CH2, CO; R1-R3 = H, OH, O(C1-C4 alkyl), etc.; n = 1, 2; W = CH2, CO; R4 = 1-piperidinyl,

2-oxo-1-piperidinyl, 1-pyrrolidinyl, etc.], useful for the treatment of the various conditions associated with post-menopausal syndrome such as osteoporosis, and uterine fibroid disease, endometriosis, and aortal smooth muscle cell proliferation, and as bone loss or resorption inhibitors and serum cholesterol levels lowering agents, were prepared and formulated. Thus, reaction of 3,9-bis[(tert-butyldimethylsilyl)oxy]-6-phenox-6-H-[1]benzothieno[3,2-c][1]benzopyran with 4-(2-piperidinoethoxy)phenylmagnesium bromide in PhMe/THF followed by removal of TBDMS groups with TBAF in THF afforded III which showed IC50 of 0.2 nM against MCF-7 breast adenocarcinoma cells proliferation.

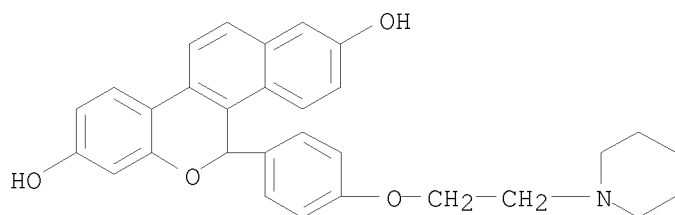
IT 188824-17-1P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of pentacyclic compds. for the treatment conditions associated with post-menopausal syndrome)

RN 188824-17-1 CAPLUS

CN 5H-Benzo[b]naphtho[2,1-d]pyran-2,8-diol,
5-[4-[2-(1-piperidinyl)ethoxy]phenyl]- (CA INDEX NAME)



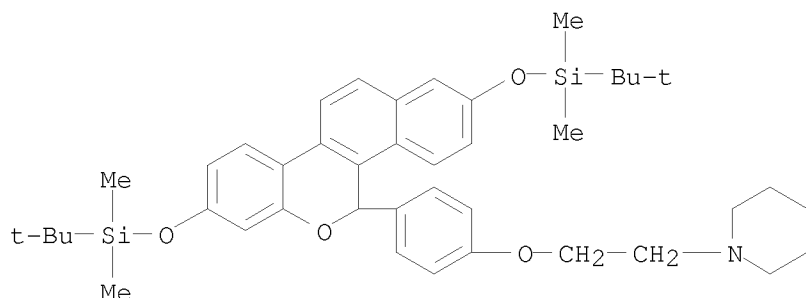
IT 188824-52-4P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of pentacyclic compds. for the treatment conditions associated with post-menopausal syndrome)

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OS.CITING REF COUNT: 7

THERE ARE 7 CAPLUS RECORDS THAT CITE THIS RECORD
(8 CITINGS)